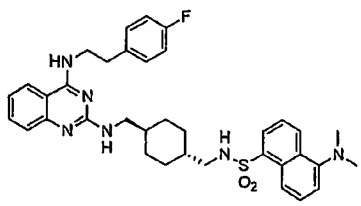
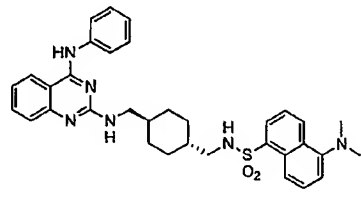
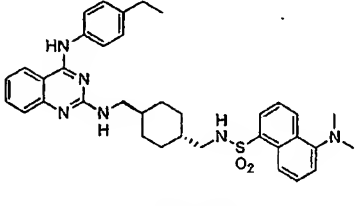
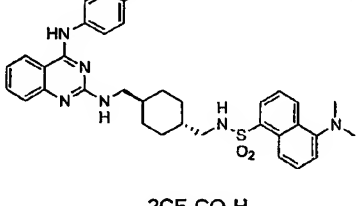
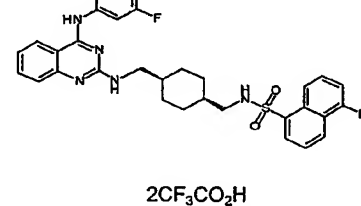
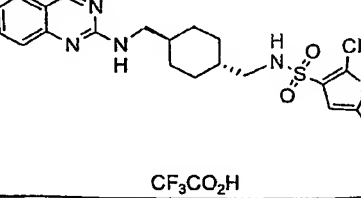
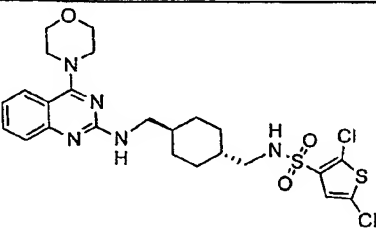
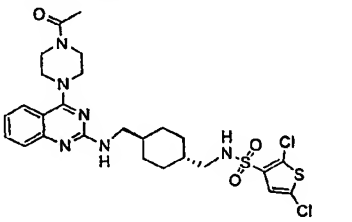
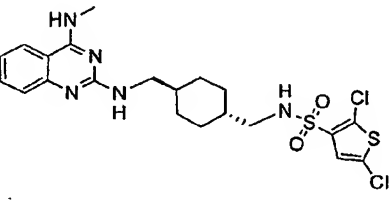
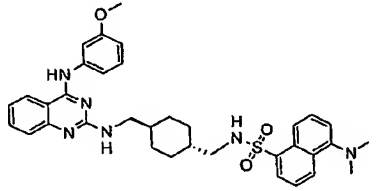
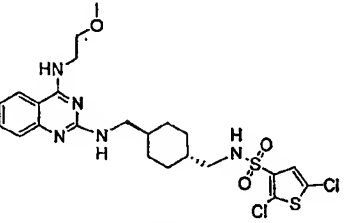
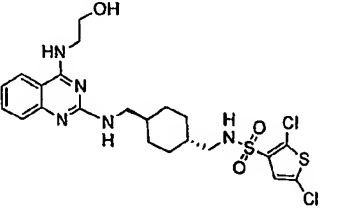
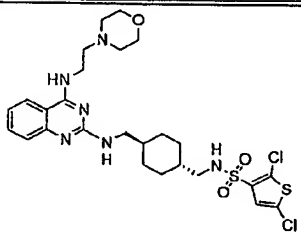
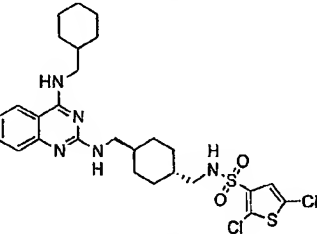
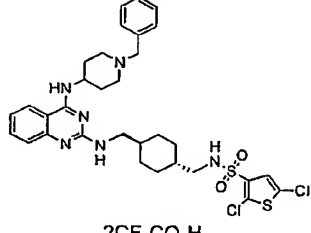
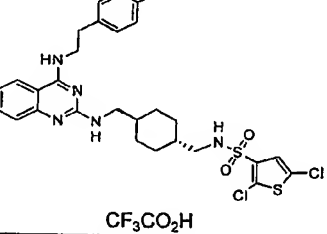
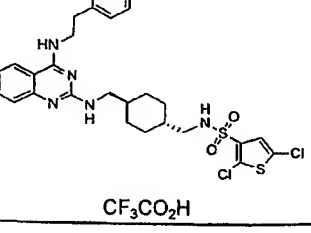
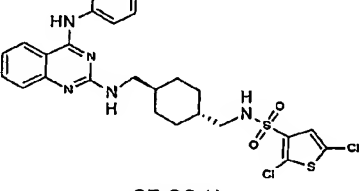
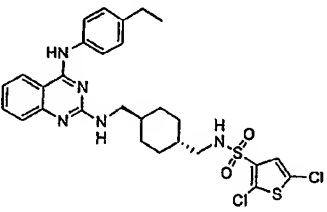
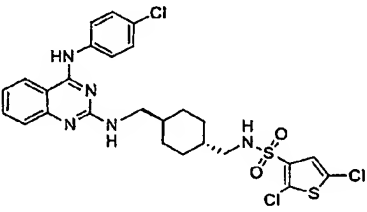
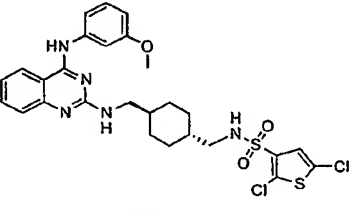
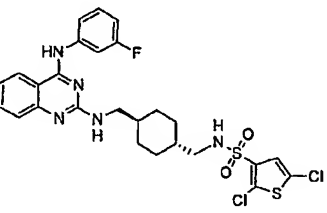
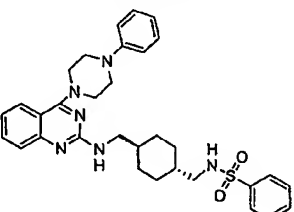
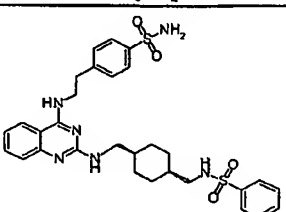
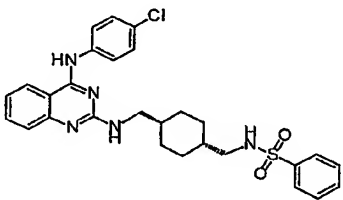
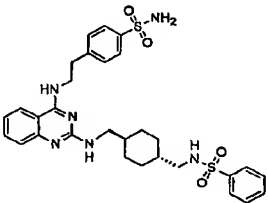
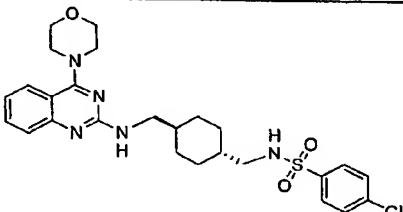
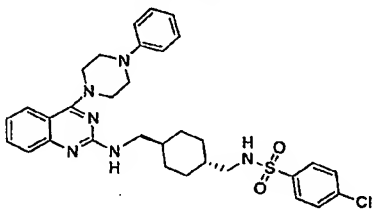
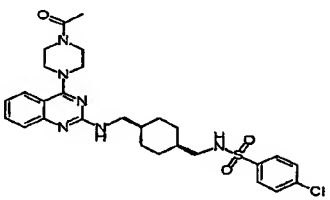
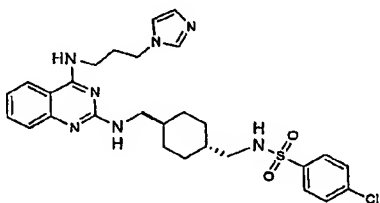


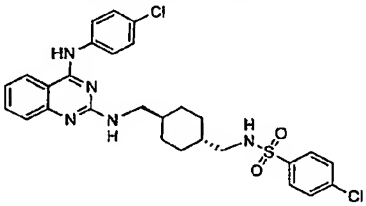
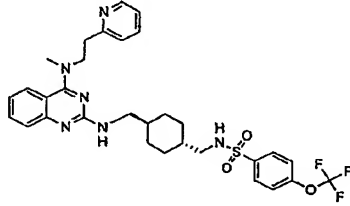
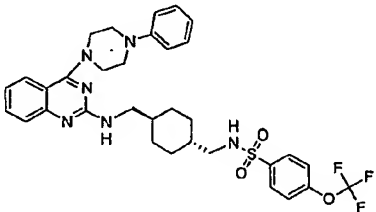
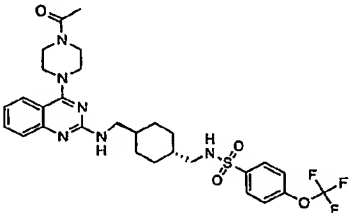
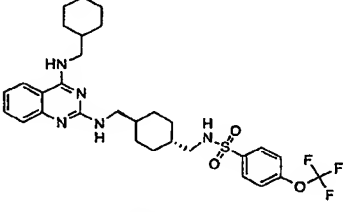
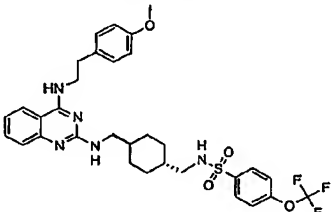
Example No.	Structure	ESI-MS	Retention Time (min)
2513	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4Cc6ccc(F)cc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	641.4 (M + H)	4.13
2514	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4Cc6ccccc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	595.4 (M + H)	3.89
2515	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4Cc6ccc(CC)cc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	623.4 (M + H)	4.20
2516	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4Cc6ccc(Cl)cc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	629.2 (M + H)	4.15
2517	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4Cc6ccccc6F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	613.2 (M + H)	4.02
2518	 <chem>CC1=CC=C(C=C1S(=O)(=O)NCC2=CC=CC=C2)CC3CCCCC3CNc4nc5ccccc5n4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	4.03

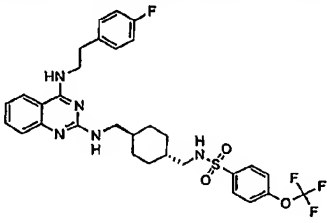
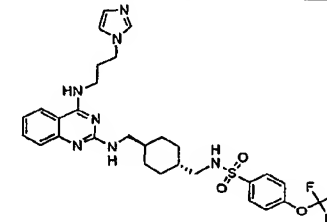
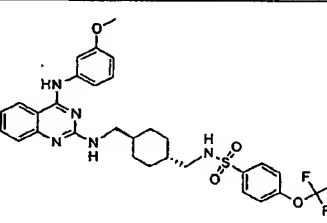
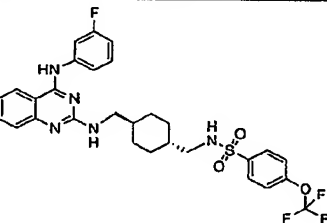
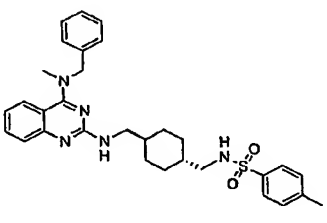
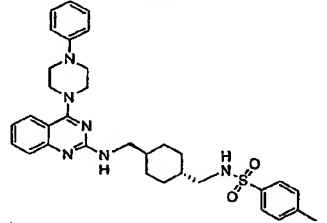
Example No.	Structure	ESI-MS	Retention Time (min)
2519	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.2 (M + H)	3.96
2520	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	611.0 (M + H)	3.69
2521	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.2 (M + H)	3.94
2522	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	625.4 (M + H)	3.94
2523	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	558.2 (M + H)	3.96
2524	 <chem>CC1(CCN(C1)c2cc3ccccc3n2)CC4(C)CCCC4NS(=O)(=O)c5cc(Cl)sc5Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	544.2 (M + H)	3.67

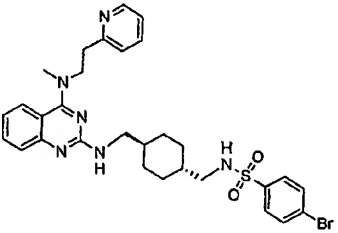
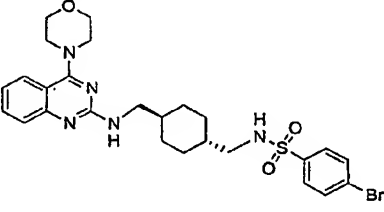
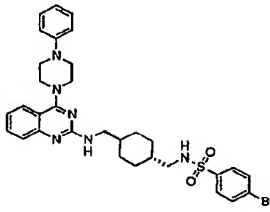
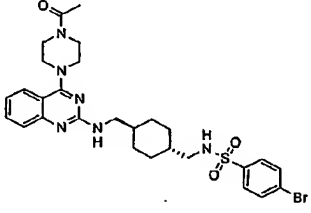
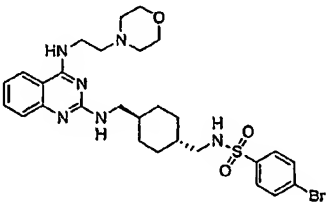
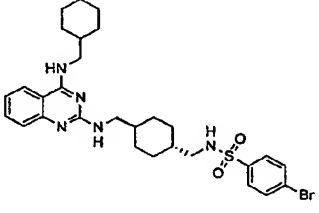
Example No.	Structure	ESI-MS	Retention Time (min)
2525	 $2\text{CF}_3\text{CO}_2\text{H}$	613.2 (M + H)	3.31
2526	 $\text{CF}_3\text{CO}_2\text{H}$	596.2 (M + H)	4.69
2527	 $2\text{CF}_3\text{CO}_2\text{H}$	673.4 (M + H)	3.57
2528	 $\text{CF}_3\text{CO}_2\text{H}$	634.4 (M + H)	4.41
2529	 $\text{CF}_3\text{CO}_2\text{H}$	622.2 (M + H)	4.45
2530	 $\text{CF}_3\text{CO}_2\text{H}$	576 (M + H)	4.25

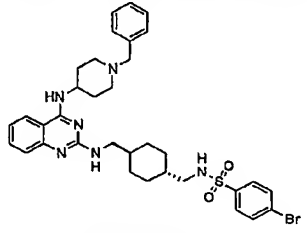
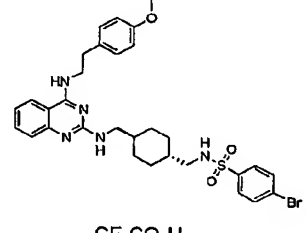
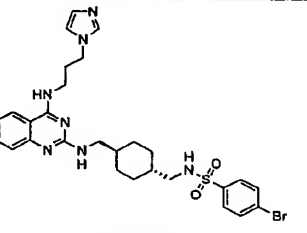
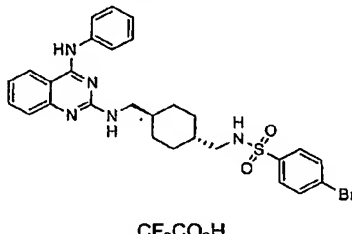
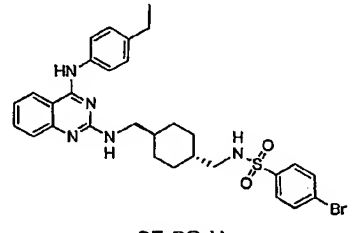
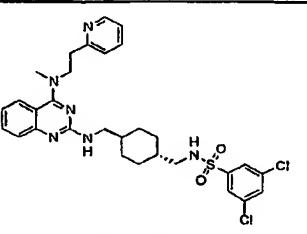
Example No.	Structure	ESI-MS	Retention Time (min)
2531	 $\text{CF}_3\text{CO}_2\text{H}$	604.4 (M + H)	4.52
2532	 $\text{CF}_3\text{CO}_2\text{H}$	610.2 (M + H)	4.40
2533	 $\text{CF}_3\text{CO}_2\text{H}$	606.4 (M + H)	4.29
2534	 $\text{CF}_3\text{CO}_2\text{H}$	594.2 (M + H)	4.27
2535	 $2\text{CF}_3\text{CO}_2\text{H}$	571.8 (M + H)	4.99
2536	 $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.43

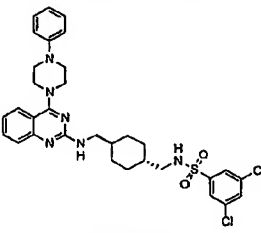
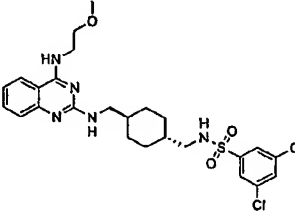
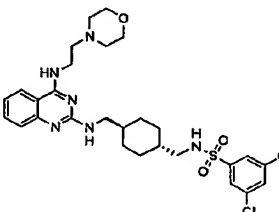
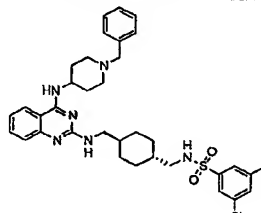
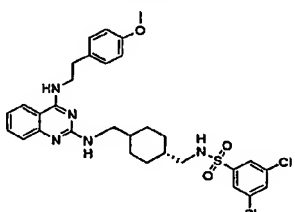
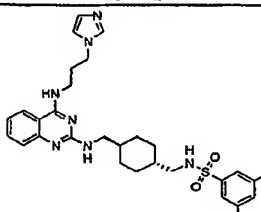
Example No.	Structure	ESI-MS	Retention Time (min)
2537	 <chem>Clc1ccc(Nc2nc3ccccc3n2CNC4CCCCC4CS(=O)(=O)c5ccc(Cl)cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	4.86
2538	 <chem>NS(=O)(=O)c1ccc(CNC2=NC3=CC=CC=C3N2CNC4CCCCC4CS(=O)(=O)c5ccc(Cl)cc5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	5.13
2539	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5CCOCC5)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	530.6 (M + H)	4.65
2540	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5CCN(C5)Cc6ccccc6)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	605.6 (M + H)	5.21
2541	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5CCN(C5)C(=O)C6CCN(C6)C)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.45
2542	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNC3=NC4=CC=CC=C4N3C5CCN(C5)CCc6ccncc6)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	568.8 (M + H)	4.09

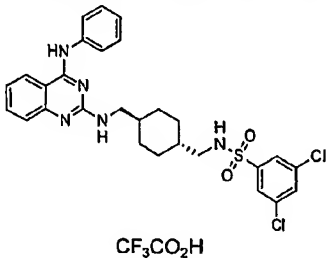
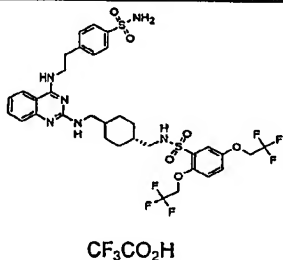
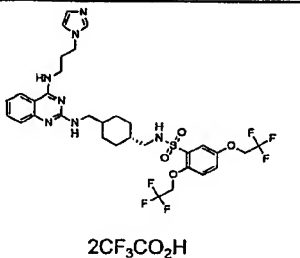
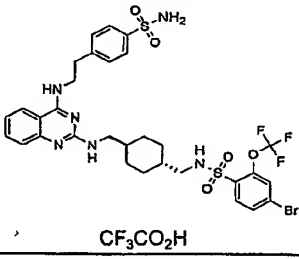
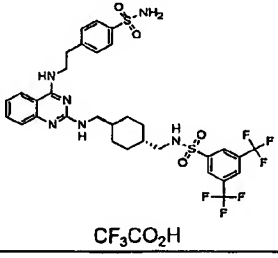
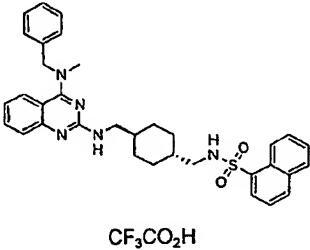
Example No.	Structure	ESI-MS	Retention Time (min)
2543	 $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.11
2544	 $2\text{CF}_3\text{CO}_2\text{H}$	629.6 (M + H)	4.37
2545	 $2\text{CF}_3\text{CO}_2\text{H}$	655.6 (M + H)	5.35
2546	 $\text{CF}_3\text{CO}_2\text{H}$	621.8 (M + H)	4.63
2547	 $\text{CF}_3\text{CO}_2\text{H}$	606.8 (M + H)	5.45
2548	 $\text{CF}_3\text{CO}_2\text{H}$	644.6 (M + H)	5.21

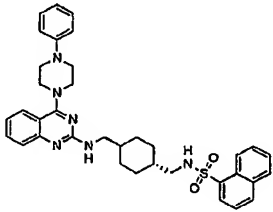
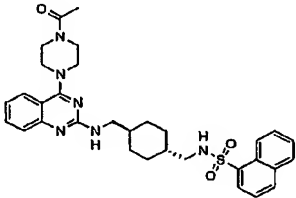
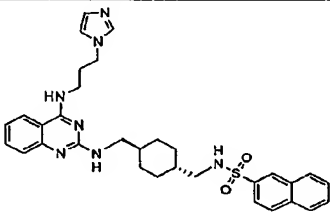
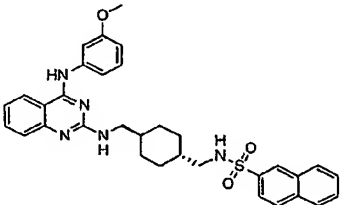
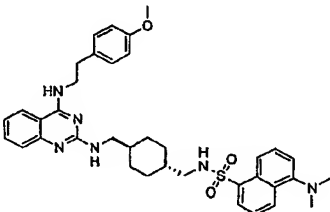
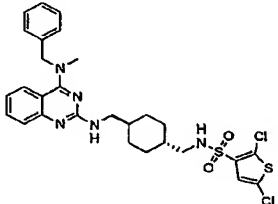
Example No.	Structure	ESI-MS	Retention Time (min)
2549	 $\text{CF}_3\text{CO}_2\text{H}$	632.6 (M + H)	5.25
2550	 $2\text{CF}_3\text{CO}_2\text{H}$	618.6 (M + H)	4.29
2551	 $\text{CF}_3\text{CO}_2\text{H}$	616.6 (M + H)	5.14
2552	 $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	5.13
2553	 $\text{CF}_3\text{CO}_2\text{H}$	544.6 (M + H)	5.03
2554	 $2\text{CF}_3\text{CO}_2\text{H}$	585.6 (M + H)	5.13

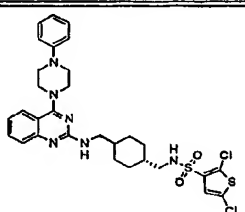
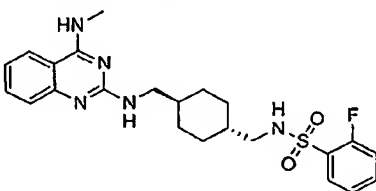
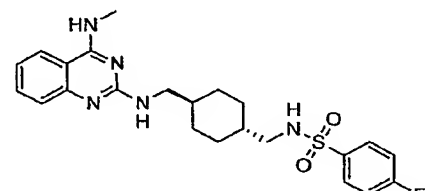
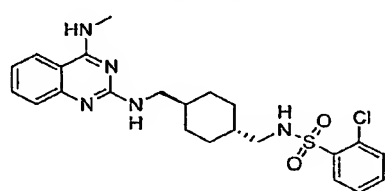
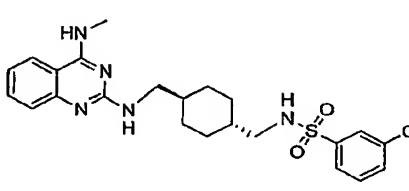
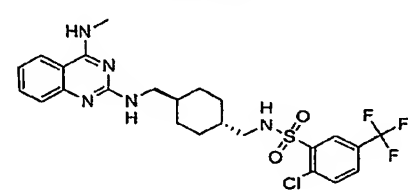
Example No.	Structure	ESI-MS	Retention Time (min)
2555	 $2\text{CF}_3\text{CO}_2\text{H}$	623.6 (M + H)	4.25
2556	 $\text{CF}_3\text{CO}_2\text{H}$	574.6 (M + H)	4.73
2557	 $2\text{CF}_3\text{CO}_2\text{H}$	649.0 (M + H)	5.25
2558	 $\text{CF}_3\text{CO}_2\text{H}$	615.0 (M + H)	4.51
2559	 $2\text{CF}_3\text{CO}_2\text{H}$	617.4 (M + H)	4.15
2560	 $\text{CF}_3\text{CO}_2\text{H}$	600.6 (M + H)	5.37

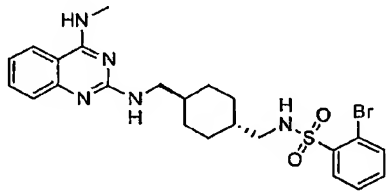
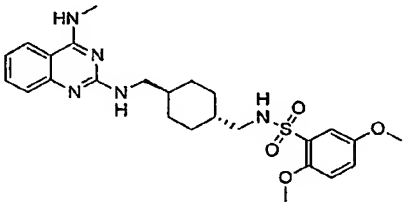
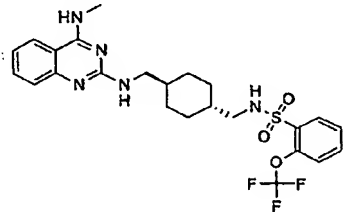
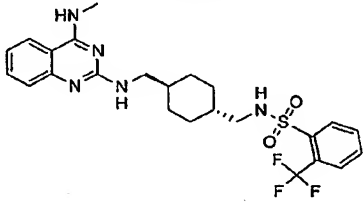
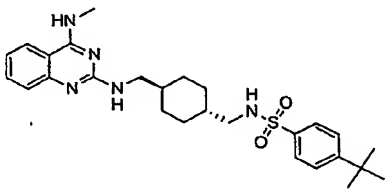
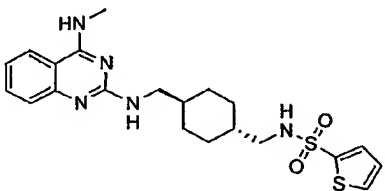
Example No.	Structure	ESI-MS	Retention Time (min)
2561	 $2\text{CF}_3\text{CO}_2\text{H}$	677.0 (M + H)	4.45
2562	 $\text{CF}_3\text{CO}_2\text{H}$	638.6 (M + H)	5.18
2563	 $2\text{CF}_3\text{CO}_2\text{H}$	612.6 (M + H)	4.16
2564	 $\text{CF}_3\text{CO}_2\text{H}$	580.0 (M + H)	5.01
2565	 $\text{CF}_3\text{CO}_2\text{H}$	608.0 (M + H)	5.26
2566	 $2\text{CF}_3\text{CO}_2\text{H}$	613.6 (M + H)	4.44

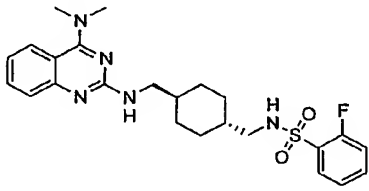
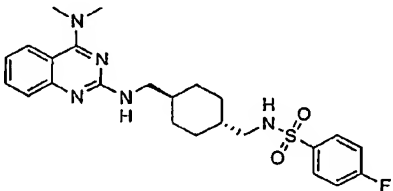
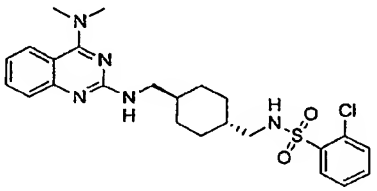
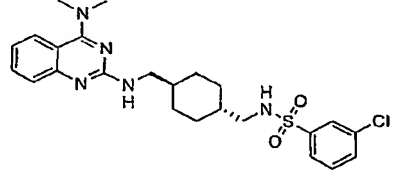
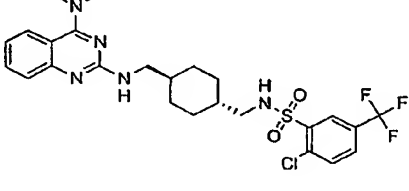
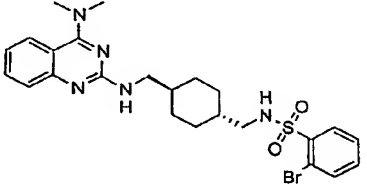
Example No.	Structure	ESI-MS	Retention Time (min)
2567	 $2\text{CF}_3\text{CO}_2\text{H}$	639.6 (M + H)	5.48
2568	 $\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	4.92
2569	 $2\text{CF}_3\text{CO}_2\text{H}$	607.8 (M + H)	4.33
2570	 $2\text{CF}_3\text{CO}_2\text{H}$	667.4 (M + H)	4.67
2571	 $\text{CF}_3\text{CO}_2\text{H}$	628.6 (M + H)	5.29
2572	 $2\text{CF}_3\text{CO}_2\text{H}$	602.6 (M + H)	4.35

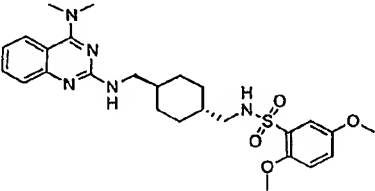
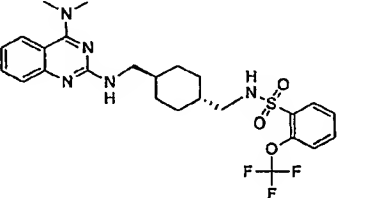
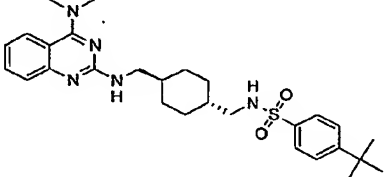
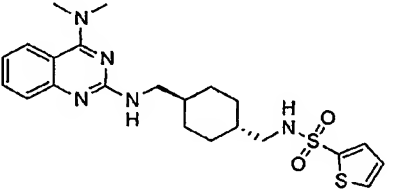
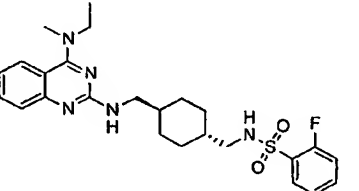
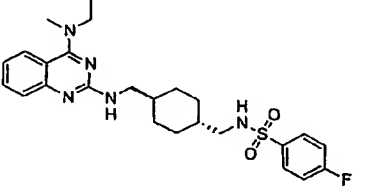
Example No.	Structure	ESI-MS	Retention Time (min)
2573	 <chem>Clc1ccc(S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5)c(c1)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.23
2574	 <chem>COc1cc(OC(F)(F)F)c(S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N5C=CC=C(C=C5)S(=O)(=O)N)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	805.4 (M + H)	4.91
2575	 <chem>COc1cc(OC(F)(F)F)c(S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N5C=CC=C(C=C5)S(=O)(=O)N)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	730.8 (M + H)	4.47
2576	 <chem>COc1cc(Br)c(S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N5C=CC=C(C=C5)S(=O)(=O)N)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	771.6 (M + H)	4.93
2577	 <chem>COc1cc(OC(F)(F)F)c(S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N5C=CC=C(C=C5)S(=O)(=O)N)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	745.6 (M + H)	5.01
2578	 <chem>c1ccc(cc1)S(=O)(=O)N[C@@H]2CCCC[C@H]2CN3C=NC4=CC=CC=C4N3C5=CC=CC=C5N5C=CC=C(C=C5)S(=O)(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	580.8 (M + H)	5.18

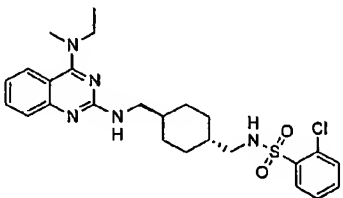
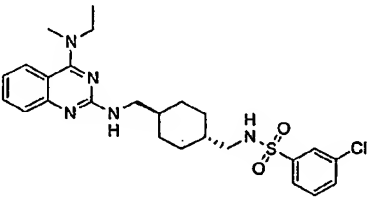
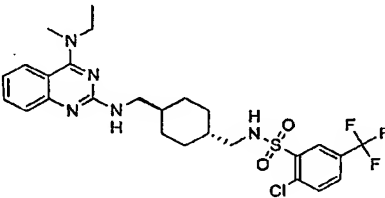
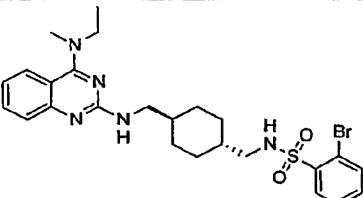
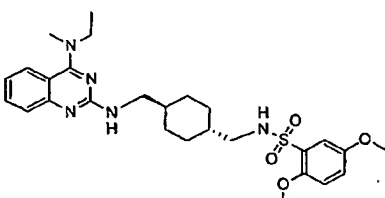
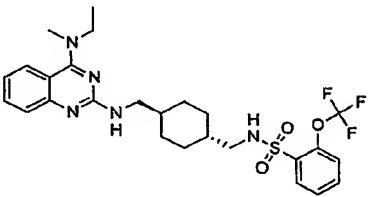
Example No.	Structure	ESI-MS	Retention Time (min)
2579	 2CF ₃ CO ₂ H	621.8 (M + H)	5.27
2580	 CF ₃ CO ₂ H	587.6 (M + H)	4.51
2581	 2CF ₃ CO ₂ H	584.6 (M + H)	4.21
2582	 CF ₃ CO ₂ H	582.8 (M + H)	5.03
2583	 CF ₃ CO ₂ H	653.8 (M + H)	4.90
2584	 CF ₃ CO ₂ H	604.6 (M + H)	5.33

Example No.	Structure	ESI-MS	Retention Time (min)
2585	 <chem>2CF3CO2H</chem>	645.6 (M + H)	5.41
2586	 <chem>CF3CO2H</chem>	458.6 (M + H)	4.39
2587	 <chem>CF3CO2H</chem>	458.6 (M + H)	4.40
2588	 <chem>CF3CO2H</chem>	474.6 (M + H)	4.39
2589	 <chem>CF3CO2H</chem>	474.6 (M + H)	4.58
2590	 <chem>CF3CO2H</chem>	542.6 (M + H)	4.79

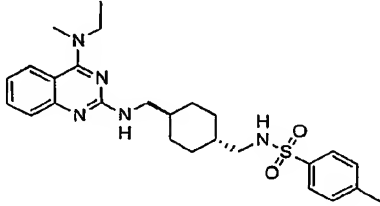
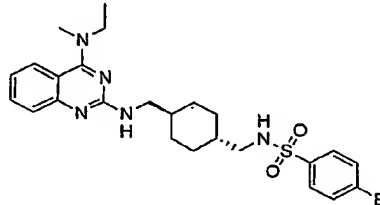
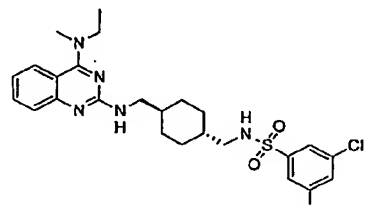
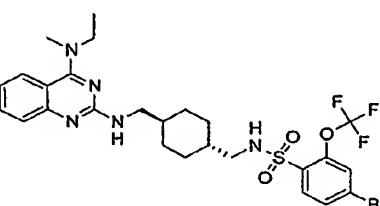
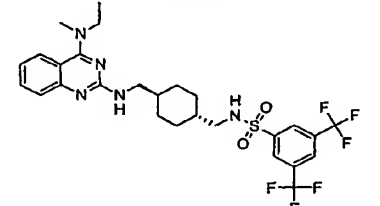
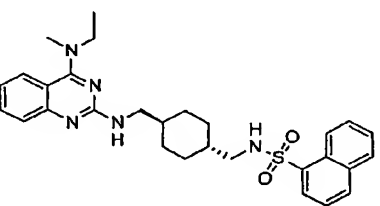
Example No.	Structure	ESI-MS	Retention Time (min)
2591	 <chem>CC1=NC2=C(N1)N=CN=C2CN[C@H]3CCCC[C@H]3CNS(=O)(=O)c4ccccc4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.51
2592	 <chem>COc1cc(OC)cc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	500.8 (M + H)	4.33
2593	 <chem>FC(F)(F)c1cc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	4.61
2594	 <chem>FC(F)(F)c1ccccc1S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.6 (M + H)	4.57
2595	 <chem>CC(C)(C)c1ccc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.87
2596	 <chem>c1cc(S)cc(S(=O)(=O)N[C@H]2CCCC[C@H]2CNc3nc4ccccc4n3)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.8 (M + H)	4.29

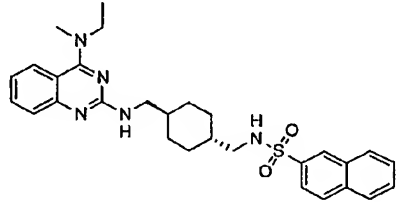
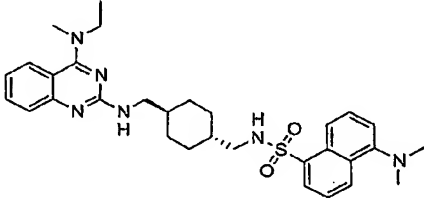
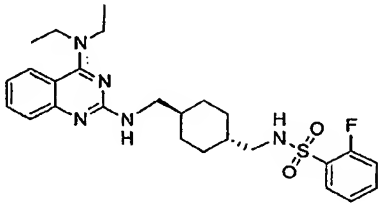
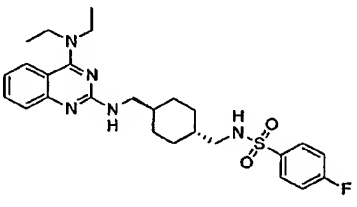
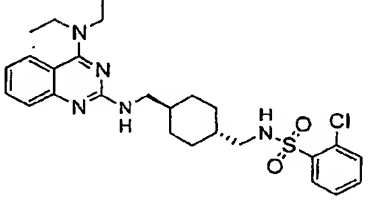
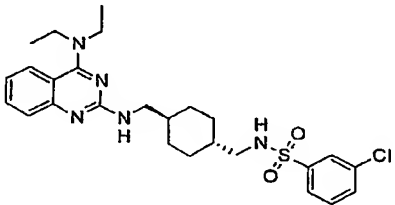
Example No.	Structure	ESI-MS	Retention Time (min)
2597	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4ccccc4F</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.47
2598	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.8 (M + H)	4.53
2599	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4ccccc4Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.55
2600	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4cccc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	487.6 (M + H)	4.65
2601	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	556.6 (M + H)	4.91
2602	 <chem>CC1=NC2=CC=CC=C2N1N(C)CNC3CCCCC3NS(=O)(=O)c4ccccc4Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	4.61

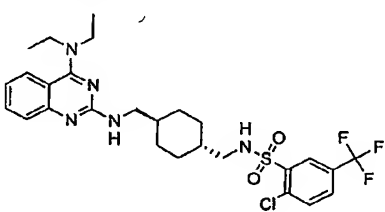
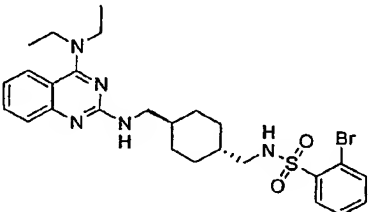
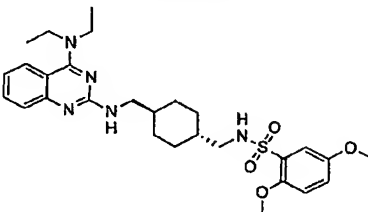
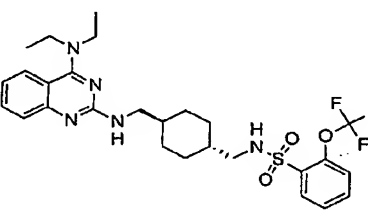
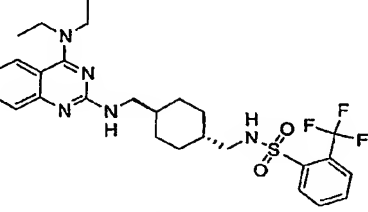
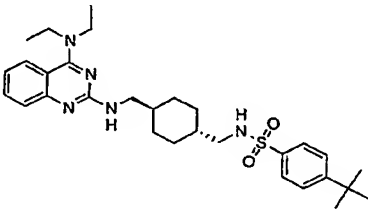
Example No.	Structure	ESI-MS	Retention Time (min)
2603	 CF ₃ CO ₂ H	514.8 (M + H)	4.43
2604	 CF ₃ CO ₂ H	538.6 (M + H)	4.80
2605	 CF ₃ CO ₂ H	510.6 (M + H)	5.00
2606	 CF ₃ CO ₂ H	460.6 (M + H)	4.40
2607	 CF ₃ CO ₂ H	486.6 (M + H)	4.60
2608	 CF ₃ CO ₂ H	484.6 (M + H)	4.64

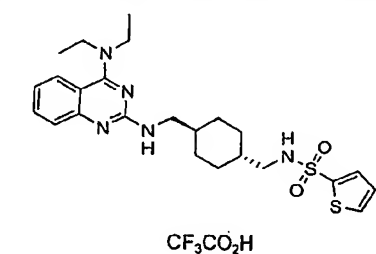
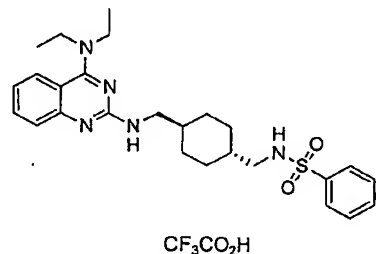
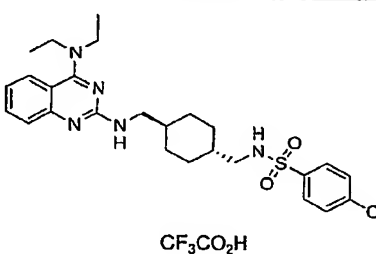
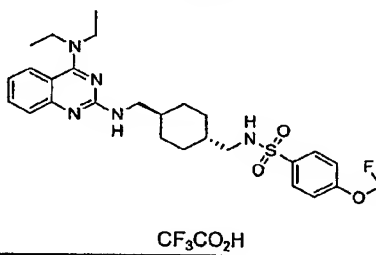
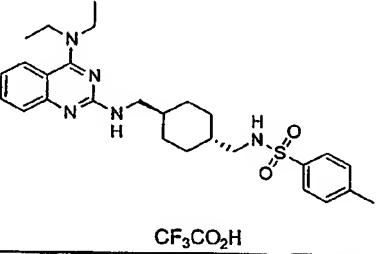
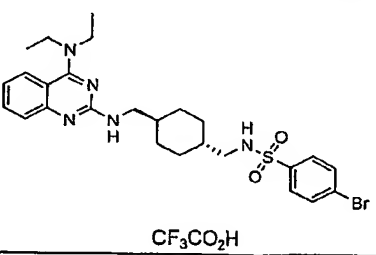
Example No.	Structure	ESI-MS	Retention Time (min)
2609	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4ccc(Cl)cc4)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	4.74
2610	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4ccc(Cl)cc4)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.86
2611	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4cc(C(F)(F)F)ccc4Cl)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.8 (M + H)	5.00
2612	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4ccccc4Br)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.0 (M + H)	4.80
2613	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4cc(OC)cc(OC)c4)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.63
2614	 <chem>CCN(C)c1nc2c(ncn2C1CC3CC(CCC3)NS(=O)(=O)c4ccccc4OC(F)(F)F)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.90

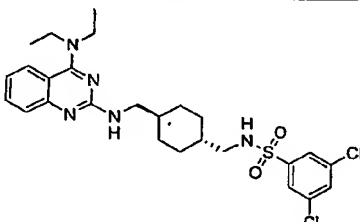
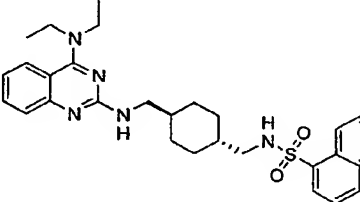
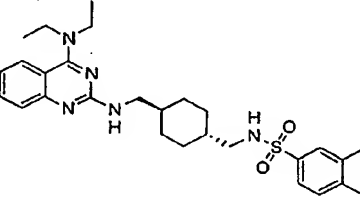
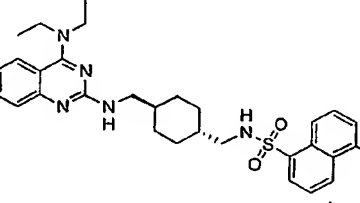
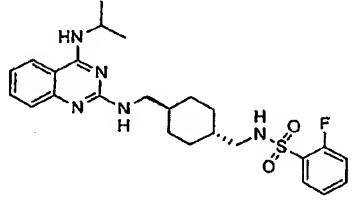
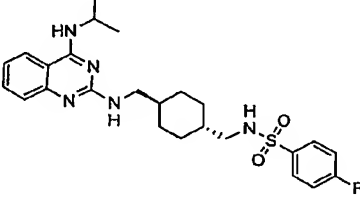
Example No.	Structure	ESI-MS	Retention Time (min)
2615	 CF ₃ CO ₂ H	536.6 (M + H)	4.82
2616	 CF ₃ CO ₂ H	524.8 (M + H)	5.07
2617	 CF ₃ CO ₂ H	474.6 (M + H)	4.55
2618	 CF ₃ CO ₂ H	468.4 (M + H)	4.59
2619	 CF ₃ CO ₂ H	502.6 (M + H)	4.81
2620	 CF ₃ CO ₂ H	552.8 (M + H)	4.94

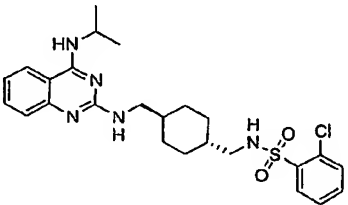
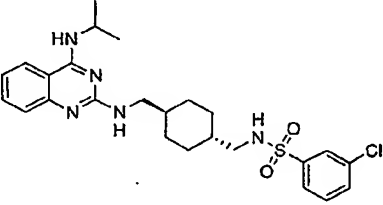
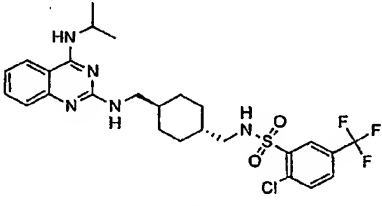
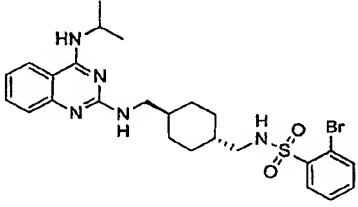
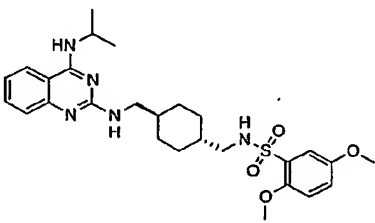
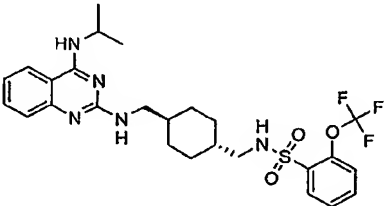
Example No.	Structure	ESI-MS	Retention Time (min)
2621	 CF ₃ CO ₂ H	482.6 (M + H)	4.73
2622	 CF ₃ CO ₂ H	546.6 (M + H)	4.85
2623	 CF ₃ CO ₂ H	536.4 (M + H)	5.08
2624	 CF ₃ CO ₂ H	630.4 (M + H)	5.11
2625	 CF ₃ CO ₂ H	604.6 (M + H)	5.16
2626	 CF ₃ CO ₂ H	518.6 (M + H)	4.75

Example No.	Structure	ESI-MS	Retention Time (min)
2627	 CF ₃ CO ₂ H	518.6 (M + H)	4.91
2628	 2CF ₃ CO ₂ H	561.6 (M + H)	4.61
2629	 CF ₃ CO ₂ H	500.8 (M + H)	4.75
2630	 CF ₃ CO ₂ H	500.2 (M + H)	4.85
2631	 CF ₃ CO ₂ H	516.6 (M + H)	4.81
2632	 CF ₃ CO ₂ H	516.6 (M + H)	4.95

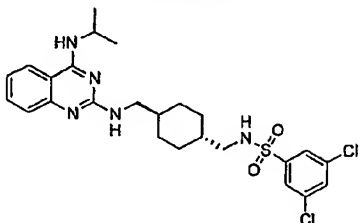
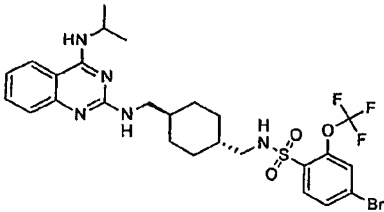
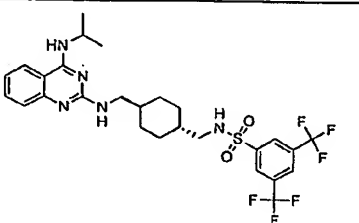
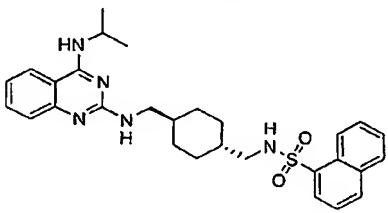
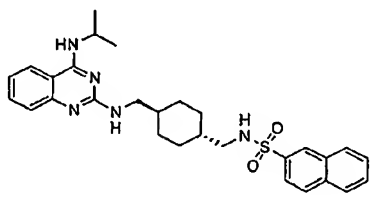
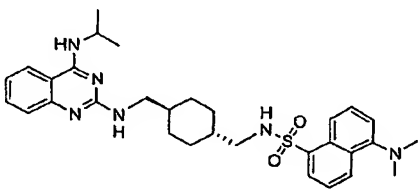
Example No.	Structure	ESI-MS	Retention Time (min)
2633	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)c(Cl)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	584.6 (M + H)	5.18
2634	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)c(Br)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.6 (M + H)	4.87
2635	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)c(OC)c(OC)c4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	542.8 (M + H)	4.80
2636	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)c(OC(F)(F)F)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.01
2637	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4cc(C(F)(F)F)c(OC(F)(F)F)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.95
2638	 <chem>CCN(CC)c1nc2c(ncn2CNC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.6 (M + H)	5.20

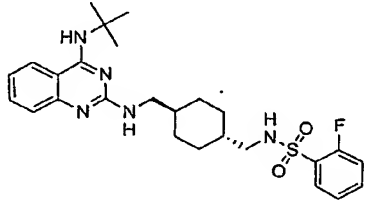
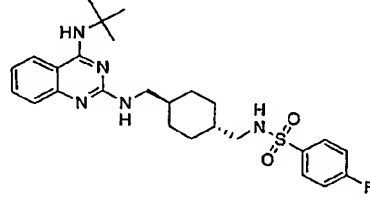
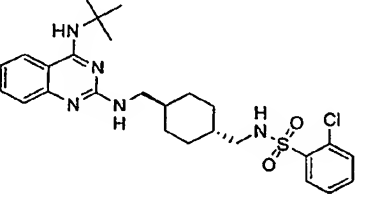
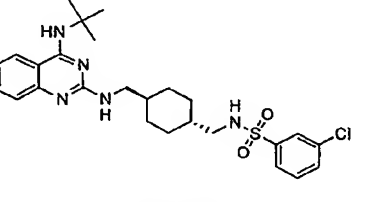
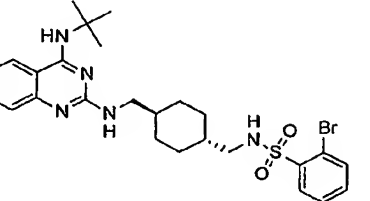
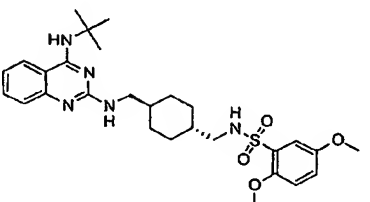
Example No.	Structure	ESI-MS	Retention Time (min)
2639	 CF ₃ CO ₂ H	488.6 (M + H)	4.65
2640	 CF ₃ CO ₂ H	482.6 (M + H)	4.73
2641	 CF ₃ CO ₂ H	516.8 (M + H)	4.97
2642	 CF ₃ CO ₂ H	566.6 (M + H)	5.12
2643	 CF ₃ CO ₂ H	496.8 (M + H)	4.89
2644	 CF ₃ CO ₂ H	560.0 (M + H)	4.98

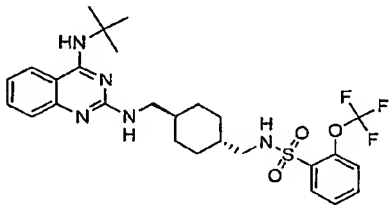
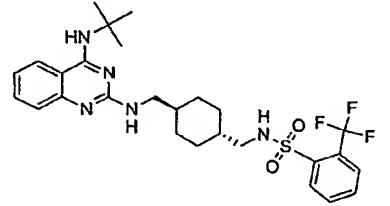
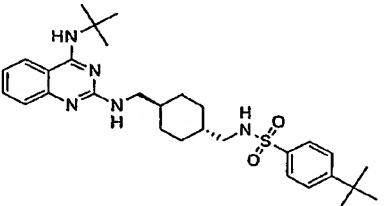
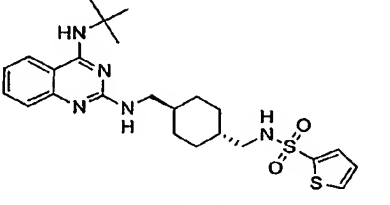
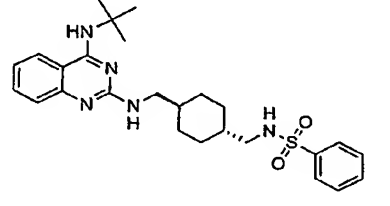
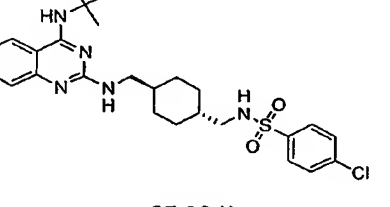
Example No.	Structure	ESI-MS	Retention Time (min)
2645	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(Cl)ccc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	5.21
2646	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cccc5ccccc45)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	4.99
2647	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccccc45)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.6 (M + H)	5.03
2648	 <chem>CCN(CC)c1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(C)cc4)C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	575.8 (M + H)	4.80
2649	 <chem>CC(C)Nc1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4cc(F)ccc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.64
2650	 <chem>CC(C)Nc1nc2c(ncn2C1CC3CCCCC3NS(=O)(=O)c4ccc(F)cc4)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	4.66

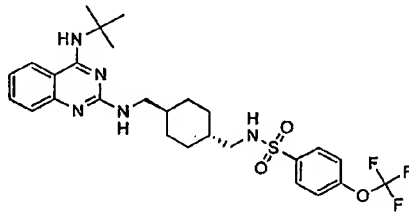
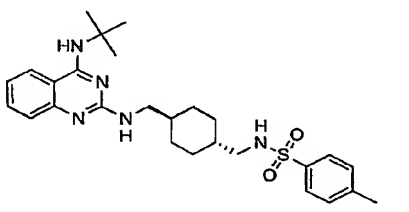
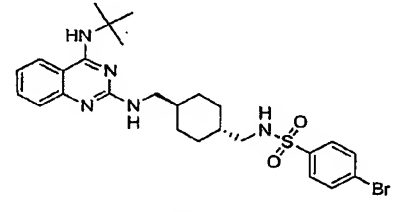
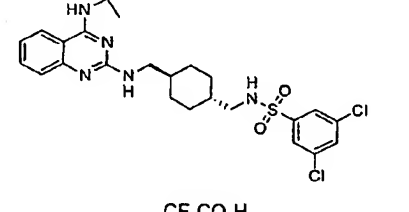
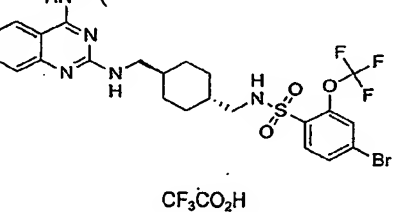
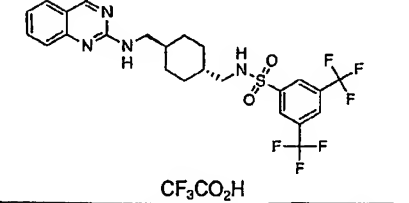
Example No.	Structure	ESI-MS	Retention Time (min)
2651	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3ccc(Cl)cc3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.72
2652	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cccc(Cl)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	502.6 (M + H)	4.87
2653	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(C(F)(F)F)cc(Cl)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	570.6 (M + H)	5.03
2654	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3ccccc3Br)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	546.6 (M + H)	4.77
2655	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(OC)cc(OC)c3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.8 (M + H)	4.68
2656	 <chem>CC(C)Nc1nc2c(ncn2C1CCN(C1)CS(=O)(=O)c3cc(OC(F)(F)F)cc3)c3ccccc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.8 (M + H)	4.89

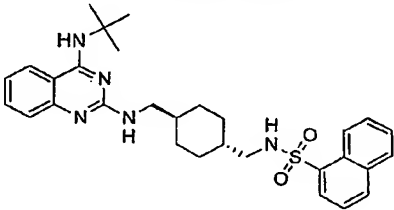
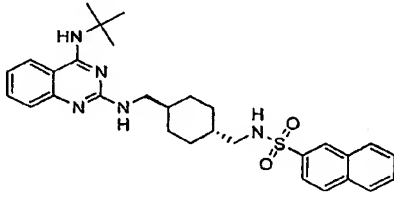
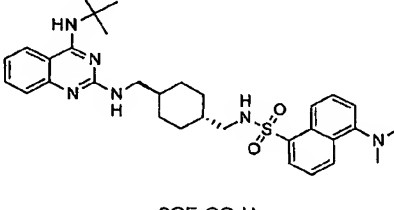
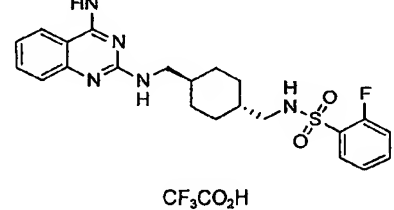
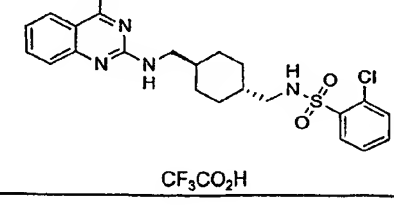
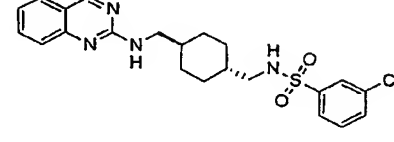
Example No.	Structure	ESI-MS	Retention Time (min)
2657	 CF ₃ CO ₂ H	536.6 (M + H)	4.85
2658	 CF ₃ CO ₂ H	524.8 (M + H)	5.15
2659	 CF ₃ CO ₂ H	474.8 (M + H)	4.63
2660	 CF ₃ CO ₂ H	468.4 (M + H)	4.61
2661	 CF ₃ CO ₂ H	502.6 (M + H)	4.86
2662	 CF ₃ CO ₂ H	546.6 (M + H)	4.64

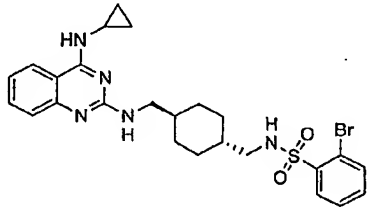
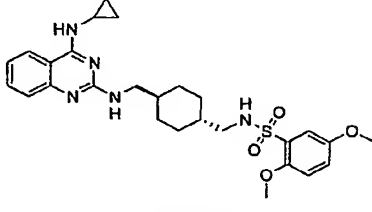
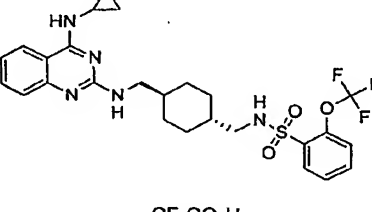
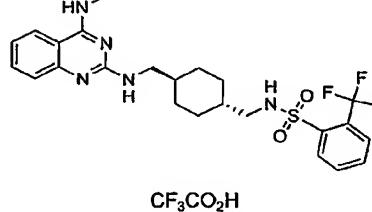
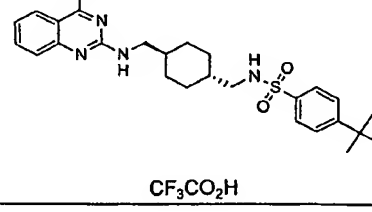
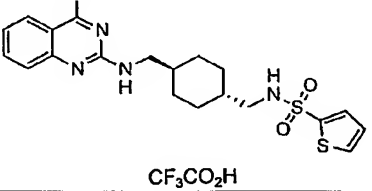
Example No.	Structure	ESI-MS	Retention Time (min)
2663	 $\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	4.81
2664	 $\text{CF}_3\text{CO}_2\text{H}$	630.4 (M + H)	4.85
2665	 $\text{CF}_3\text{CO}_2\text{H}$	604.6 (M + H)	4.87
2666	 $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.67
2667	 $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.90
2668	 $2\text{CF}_3\text{CO}_2\text{H}$	561.6 (M + H)	4.64

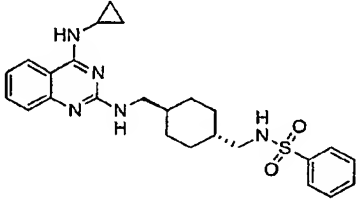
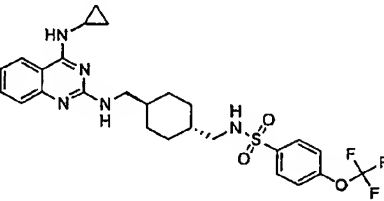
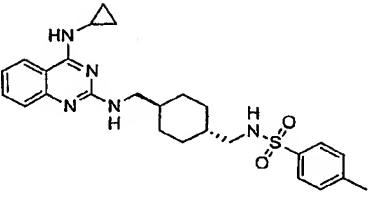
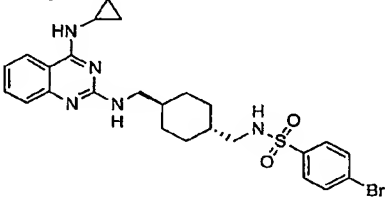
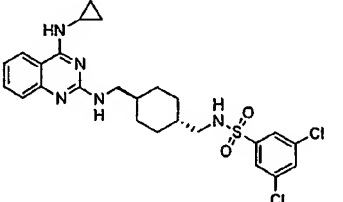
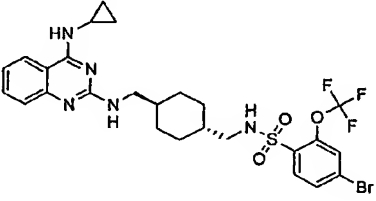
Example No.	Structure	ESI-MS	Retention Time (min)
2669	 CF ₃ CO ₂ H	500.8 (M + H)	4.73
2670	 CF ₃ CO ₂ H	500.8 (M + H)	4.74
2671	 CF ₃ CO ₂ H	516.6 (M + H)	4.89
2672	 CF ₃ CO ₂ H	516.6 (M + H)	4.93
2673	 CF ₃ CO ₂ H	560.0 (M + H)	4.89
2674	 CF ₃ CO ₂ H	542.8 (M + H)	4.76

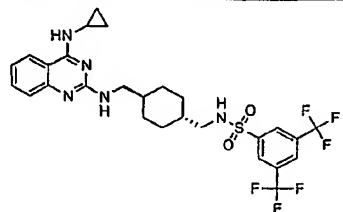
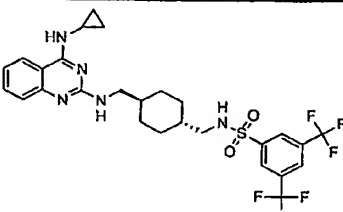
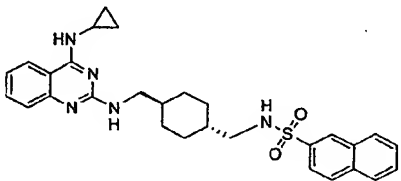
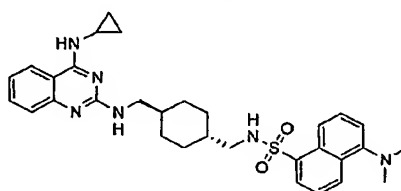
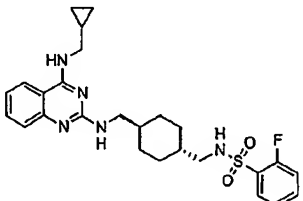
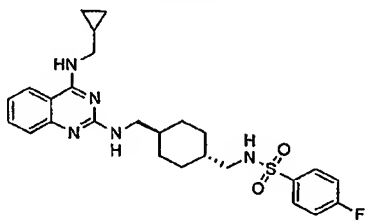
Example No.	Structure	ESI-MS	Retention Time (min)
2675	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4OC(F)(F)F)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.6 (M + H)	5.03
2676	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4C(F)F)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.8 (M + H)	4.96
2677	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccc(C(C)(C)C)cc4)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	538.8 (M + H)	5.25
2678	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4S)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.6 (M + H)	4.67
2679	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccccc4)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.71
2680	 <chem>CC(C)(C)Nc1nc2c(ncn2C1CCNCC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4)c5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.6 (M + H)	4.95

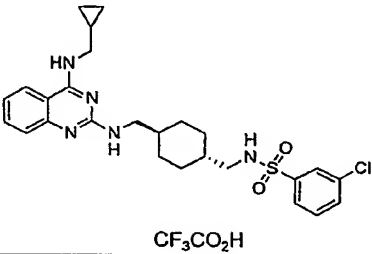
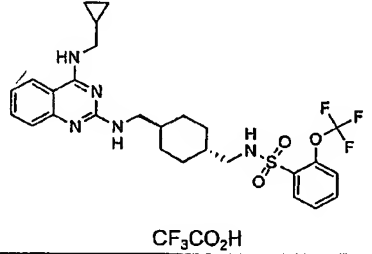
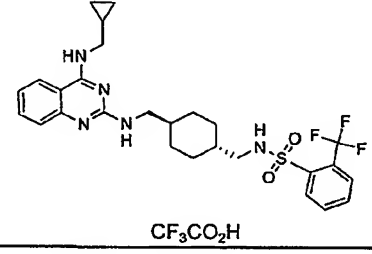
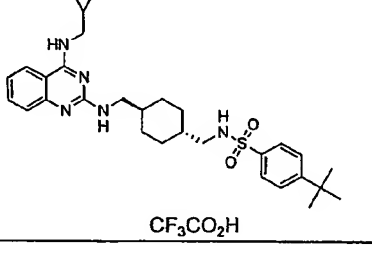
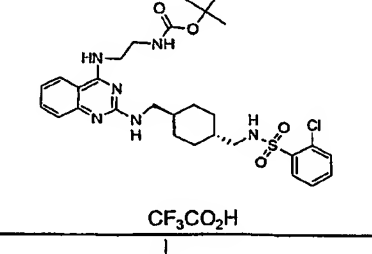
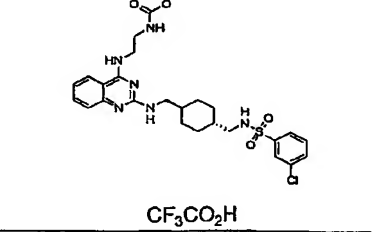
Example No.	Structure	ESI-MS	Retention Time (min)
2681	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5ccc(OC(F)(F)F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	566.8 (M + H)	5.07
2682	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5ccc(C)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.8 (M + H)	4.83
2683	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5ccc(Br)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	560.6 (M + H)	5.01
2684	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5cc(Cl)cc(Cl)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	5.07
2685	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5cc(Br)cc(OC(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.6 (M + H)	5.29
2686	 <chem>CC1(C)NC2=NC3=CC=CC=C3N=C2N1CC4CCCCC4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	618.6 (M + H)	5.25

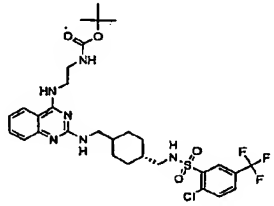
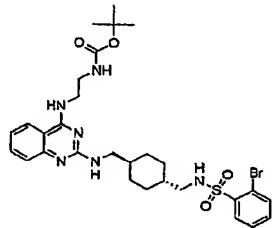
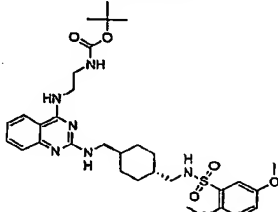
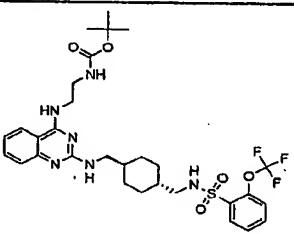
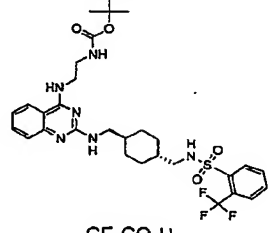
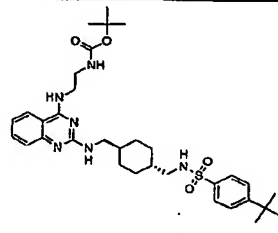
Example No.	Structure	ESI-MS	Retention Time (min)
2687	 <p>CF₃CO₂H</p>	532.6 (M + H)	5.01
2688	 <p>CF₃CO₂H</p>	532.6 (M + H)	5.04
2689	 <p>2CF₃CO₂H</p>	575.8 (M + H)	4.75
2690	 <p>CF₃CO₂H</p>	484.6 (M + H)	4.51
2691	 <p>CF₃CO₂H</p>	500.8 (M + H)	4.59
2692	 <p>CF₃CO₂H</p>	500.8 (M + H)	4.71

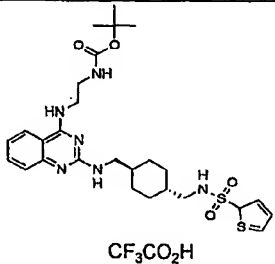
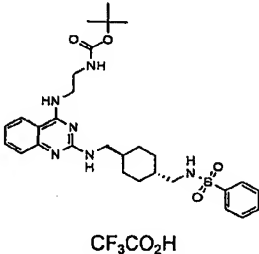
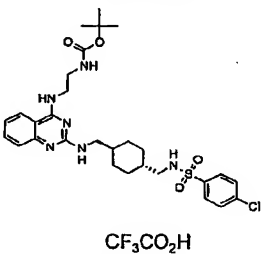
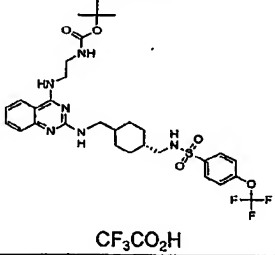
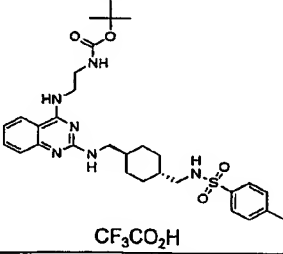
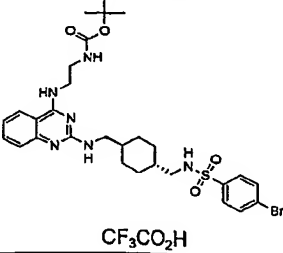
Example No.	Structure	ESI-MS	Retention Time (min)
2693	 CF ₃ CO ₂ H	544.6 (M + H)	4.63
2694	 CF ₃ CO ₂ H	526.8 (M + H)	4.55
2695	 CF ₃ CO ₂ H	550.6 (M + H)	4.79
2696	 CF ₃ CO ₂ H	534.6 (M + H)	4.69
2697	 CF ₃ CO ₂ H	522.4 (M + H)	5.03
2698	 CF ₃ CO ₂ H	472.8 (M + H)	4.43

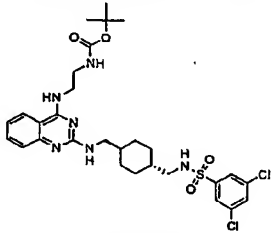
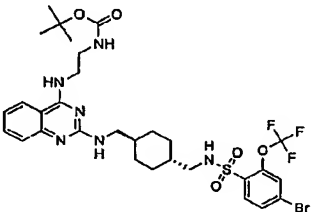
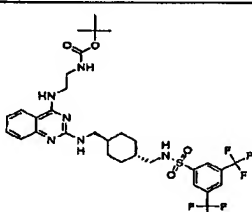
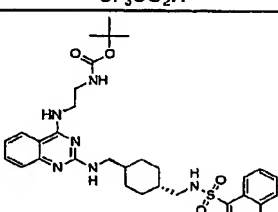
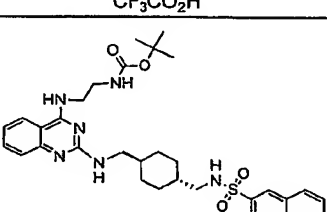
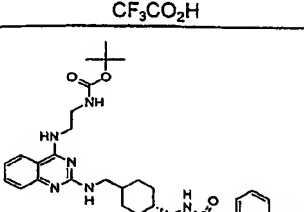
Example No.	Structure	ESI-MS	Retention Time (min)
2699	 <chem>CF3CO2H</chem>	466.6 (M + H)	4.50
2700	 <chem>CF3CO2H</chem>	550.6 (M + H)	4.87
2701	 <chem>CF3CO2H</chem>	480.6 (M + H)	4.65
2702	 <chem>CF3CO2H</chem>	544.6 (M + H)	4.75
2703	 <chem>CF3CO2H</chem>	534.6 (M + H)	4.90
2704	 <chem>CF3CO2H</chem>	628.6 (M + H)	5.08

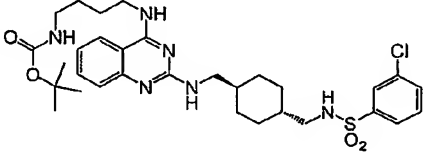
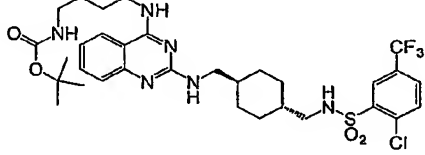
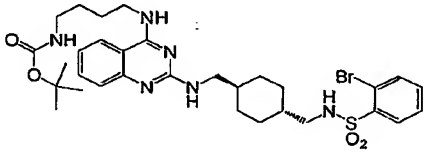
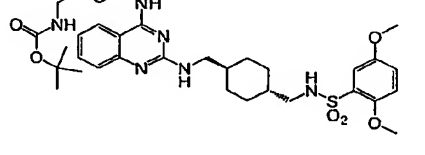
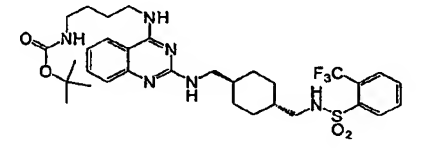
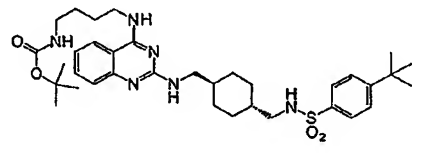
Example No.	Structure	ESI-MS	Retention Time (min)
2705	 <chem>CC1(C)Nc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	602.6 (M + H)	5.10
2706	 <chem>CC1(C)Nc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5cc(C(F)(F)F)cc(C(F)(F)F)c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.71
2707	 <chem>CC1(C)Nc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc6ccccc6c5</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.8 (M + H)	4.81
2708	 <chem>CC1(C)Nc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc6cc(C)ccc6c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.50
2709	 <chem>CC1(C)CNc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccccc5F</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.64
2710	 <chem>CC1(C)CNc2nc3ccccc3nc2N1CC[C@H]4CCCC[C@H]4NS(=O)(=O)c5ccc(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.8 (M + H)	4.73

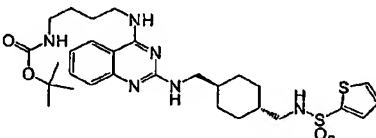
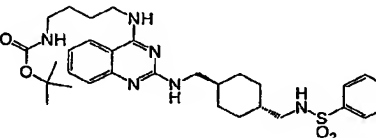
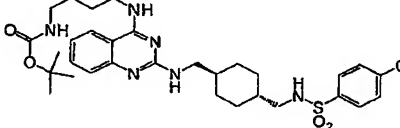
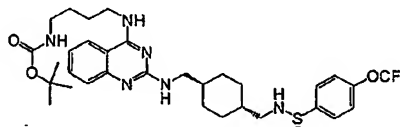
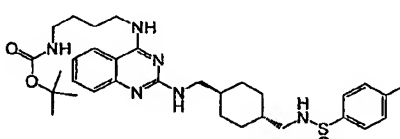
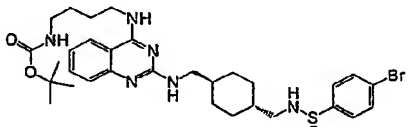
Example No.	Structure	ESI-MS	Retention Time (min)
2711	 <chem>Clc1ccc(cc1)S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)C5CCCC5</chem> $\text{CF}_3\text{CO}_2\text{H}$	514.8 (M + H)	4.87
2712	 <chem>Fc1cc(ccc1S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)C5CCCC5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	564.6 (M + H)	4.93
2713	 <chem>Fc1cc(ccc1S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)C5CCCC5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	548.6 (M + H)	4.87
2714	 <chem>CC(C)(C)c1ccc(cc1S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)C5CCCC5)</chem> $\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	5.19
2715	 <chem>Clc1ccc(cc1S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)CCNC(=O)OC(C)(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.76
2716	 <chem>Clc1ccc(cc1S(=O)(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C4)CCNC(=O)OC(C)(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	603.4 (M + H)	4.87

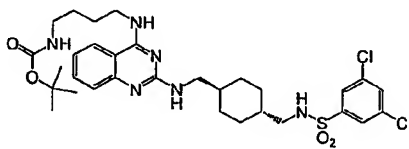
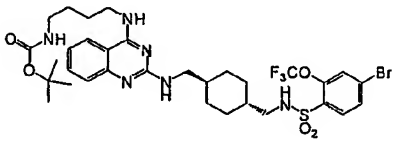
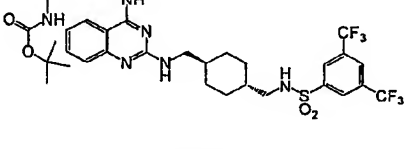
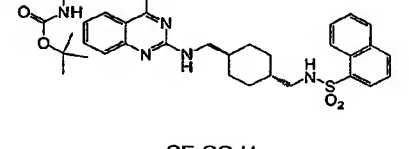
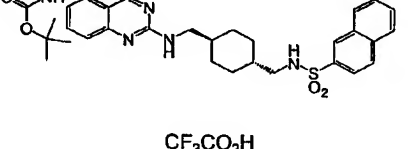
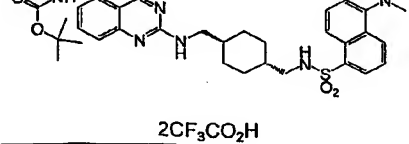
Example No.	Structure	ESI-MS	Retention Time (min)
2717	 $\text{CF}_3\text{CO}_2\text{H}$	671.6 (M + H)	5.05
2718	 $\text{CF}_3\text{CO}_2\text{H}$	647.6 (M + H)	4.79
2719	 $\text{CF}_3\text{CO}_2\text{H}$	629.8 (M + H)	4.67
2720	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	4.91
2721	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	4.85
2722	 $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	5.14

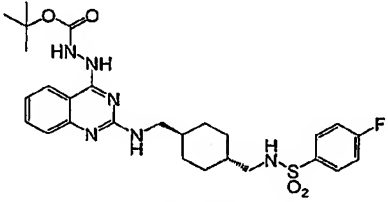
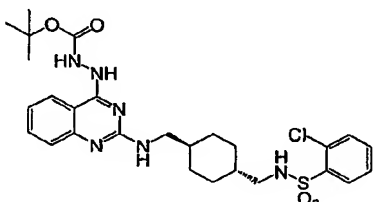
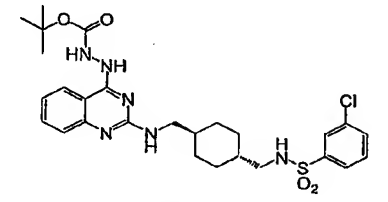
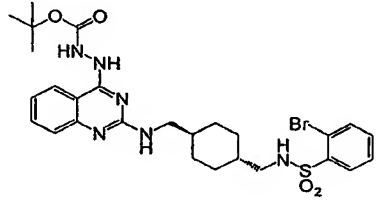
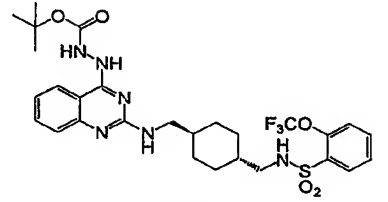
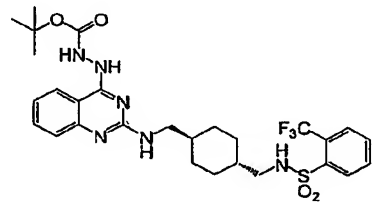
Example No.	Structure	ESI-MS	Retention Time (min)
2723	 $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.63
2724	 $\text{CF}_3\text{CO}_2\text{H}$	569.8 (M + H)	4.66
2725	 $\text{CF}_3\text{CO}_2\text{H}$	603.8 (M + H)	4.88
2726	 $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.01
2727	 $\text{CF}_3\text{CO}_2\text{H}$	583.8 (M + H)	4.77
2728	 $\text{CF}_3\text{CO}_2\text{H}$	647 (M + H)	4.92

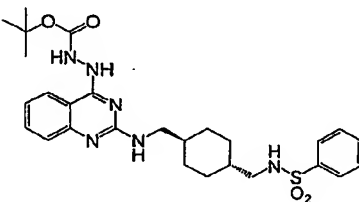
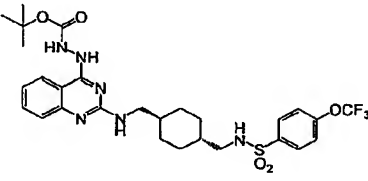
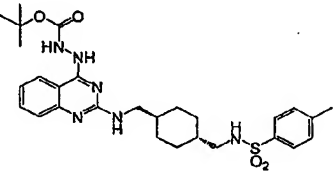
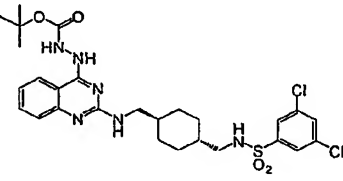
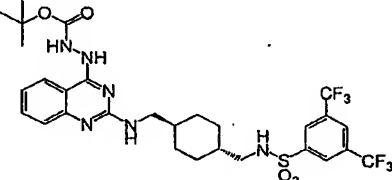
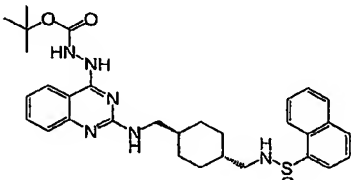
Example No.	Structure	ESI-MS	Retention Time (min)
2729	 $\text{CF}_3\text{CO}_2\text{H}$	637.8 (M + H)	5.13
2730	 $\text{CF}_3\text{CO}_2\text{H}$	731.6 (M + H)	5.19
2731	 $\text{CF}_3\text{CO}_2\text{H}$	705.8 (M + H)	5.22
2732	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.91
2733	 $\text{CF}_3\text{CO}_2\text{H}$	619.8 (M + H)	4.93
2734	 $2\text{CF}_3\text{CO}_2\text{H}$	663.0 (M + H)	4.67

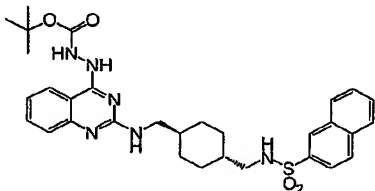
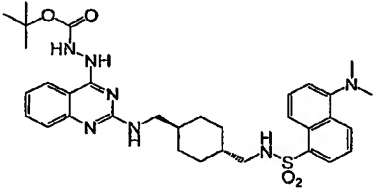
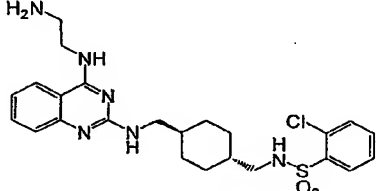
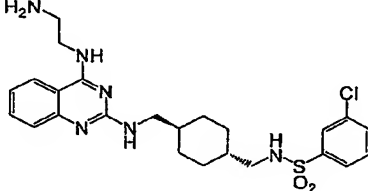
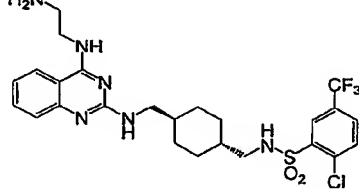
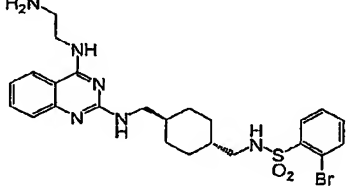
Example No.	Structure	ESI-MS	Retention Time (min)
2735	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccc(Cl)cc5)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	631.8 (M + H)	5.01
2736	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccc(C(F)(F)F)cc5Cl)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	699.0 (M + H)	5.19
2737	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccccc5Br)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	675.8 (M + H)	4.95
2738	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccc(OC)cc5OC)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	657.8 (M + H)	4.81
2739	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccccc5C(F)(F)F)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	4.97
2740	 <chem>CC1(C)OC(=O)N[C@H]1c2nc3c(ncn3C4CCCCC4NS(=O)(=O)c5ccc(C(C)(C)C)cc5)c6ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	653.8 (M + H)	5.27

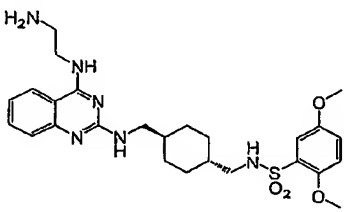
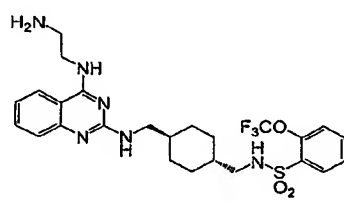
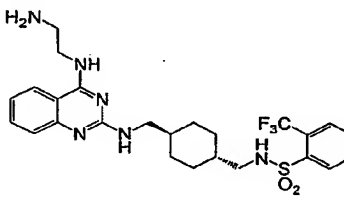
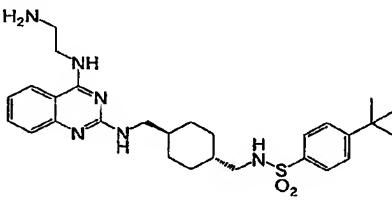
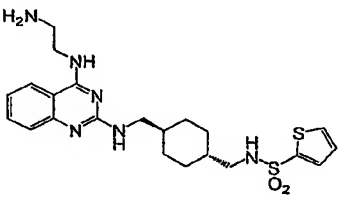
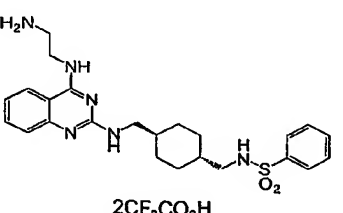
Example No.	Structure	ESI-MS	Retention Time (min)
2741	 CF ₃ CO ₂ H	603.4 (M + H)	4.77
2742	 CF ₃ CO ₂ H	597.8 (M + H)	4.79
2743	 CF ₃ CO ₂ H	631.8 (M + H)	5.02
2744	 CF ₃ CO ₂ H	681.8 (M + H)	5.14
2745	 CF ₃ CO ₂ H	611.8 (M + H)	4.93
2746	 CF ₃ CO ₂ H	675.0 (M + H)	5.05

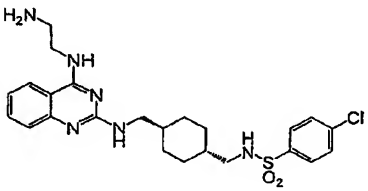
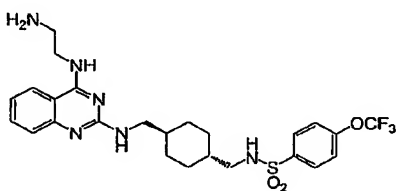
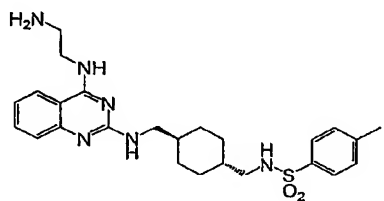
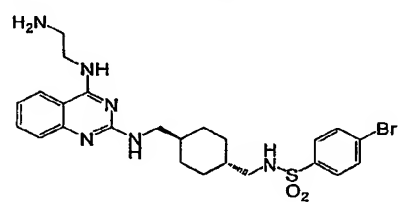
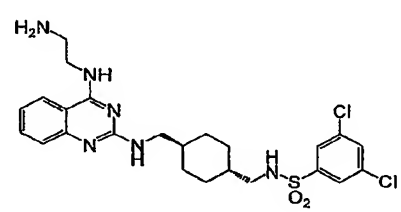
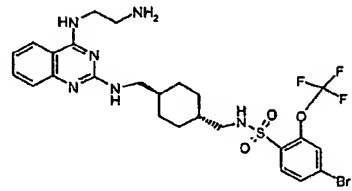
Example No.	Structure	ESI-MS	Retention Time (min)
2747	 $\text{CF}_3\text{CO}_2\text{H}$	665.8 (M + H)	5.29
2748	 $\text{CF}_3\text{CO}_2\text{H}$	759.6 (M + H)	5.31
2749	 $\text{CF}_3\text{CO}_2\text{H}$	733.8 (M + H)	5.36
2750	 $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.05
2751	 $\text{CF}_3\text{CO}_2\text{H}$	647.8 (M + H)	5.08
2752	 $2\text{CF}_3\text{CO}_2\text{H}$	691.0 (M + H)	4.89

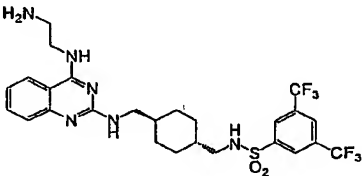
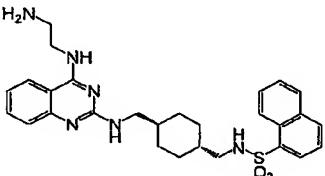
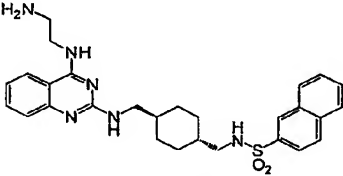
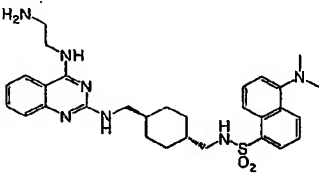
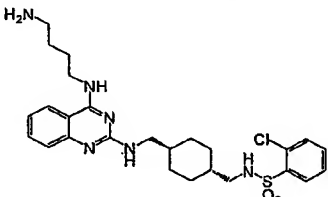
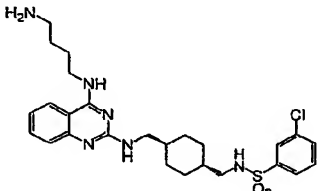
Example No.	Structure	ESI-MS	Retention Time (min)
2753	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4ccc(F)cc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	559.6 (M + H)	4.51
2754	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4ccc(Cl)cc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.57
2755	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4cc(Cl)ccc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	575.6 (M + H)	4.69
2756	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4cc(Br)ccc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	619.6 (M + H)	4.63
2757	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4ccc(cc4)C(F)(F)F)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.72
2758	 <chem>CC(C)(C)OC(=O)NNc1nc2c(ncn2C1Cc3ccc(cc3)NS(=O)(=O)c4cc(C(F)(F)F)ccc4)cc5ccccc15</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.67

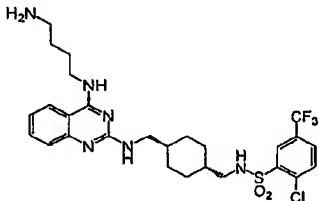
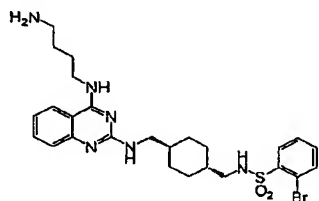
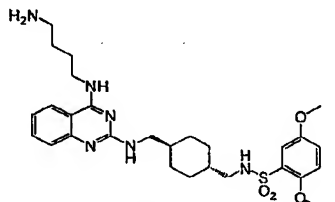
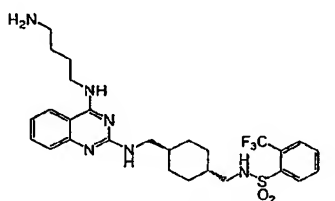
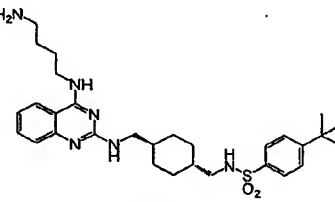
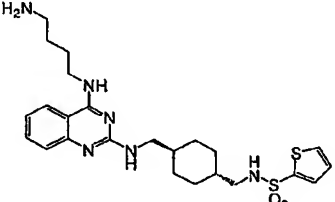
Example No.	Structure	ESI-MS	Retention Time (min)
2759	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	541.8 (M + H)	4.45
2760	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	625.8 (M + H)	4.38
2761	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4ccc(C)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	555.8 (M + H)	4.57
2762	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	609.8 (M + H)	4.94
2763	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4cc(C(F)(F)F)cc(C(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	677.8 (M + H)	5.05
2764	 <chem>CC(C)(C)OC(=O)NNc1nc2c(nc1c2)NCC3CCCCC3CNS(=O)(=O)c4c5ccccc5cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.73

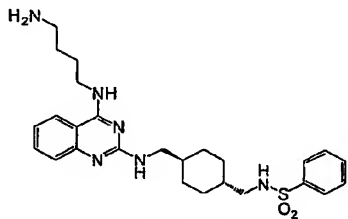
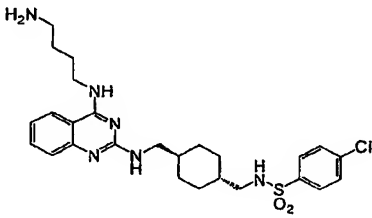
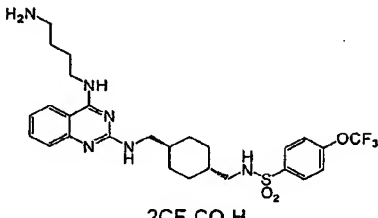
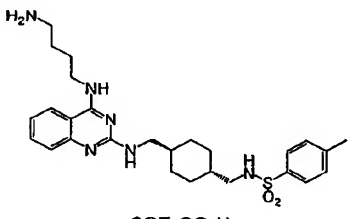
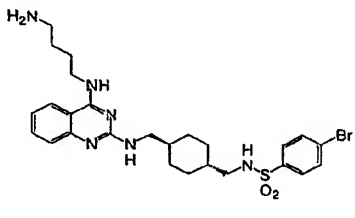
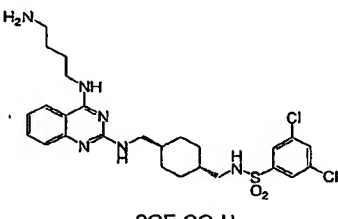
Example No.	Structure	ESI-MS	Retention Time (min)
2765	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	591.6 (M + H)	4.75
2766	 <chem>CC(C)(C)OC(=O)NNc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	635.0 (M + H)	4.47
2767	 <chem>NCCNC(=O)Nc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccccc4Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.83
2768	 <chem>NCCNC(=O)Nc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.99
2769	 <chem>NCCNC(=O)Nc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4cc(Cl)cc(C(F)(F)F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	571.6 (M + H)	4.16
2770	 <chem>NCCNC(=O)Nc1nc2ccccc2n1CNC3CCCCC3CNS(=O)(=O)c4ccc(Br)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	3.85

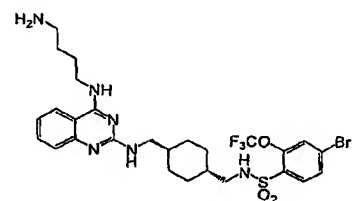
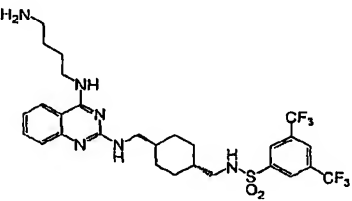
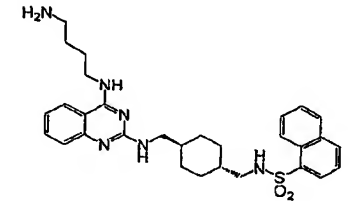
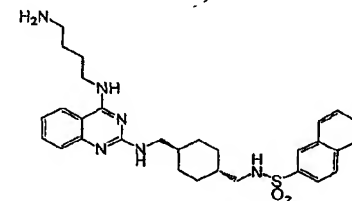
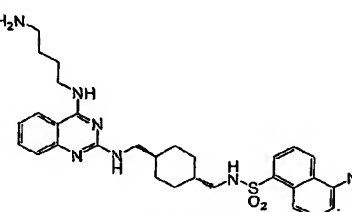
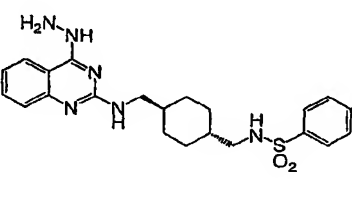
Example No.	Structure	ESI-MS	Retention Time (min)
2771	 <chem>COc1ccc(cc1)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	529.6 (M + H)	3.75
2772	 <chem>FC(F)(F)c1ccc(cc1)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	553.8 (M + H)	3.99
2773	 <chem>FC(F)(F)c1cccc(c1)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	537.6 (M + H)	3.93
2774	 <chem>CC(C)(C)c1ccc(cc1)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	525.8 (M + H)	4.22
2775	 <chem>c1ccsc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	3.64
2776	 <chem>c1ccccc1S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3CNCCN</chem> $2\text{CF}_3\text{CO}_2\text{H}$	469.6 (M + H)	3.71

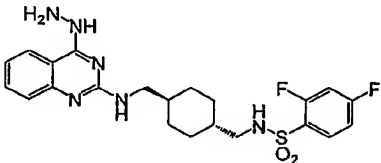
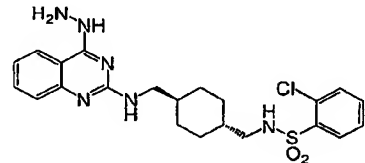
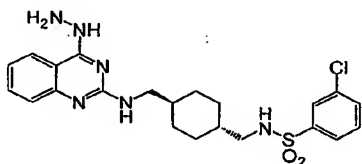
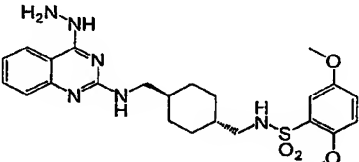
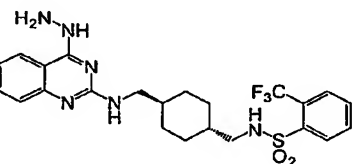
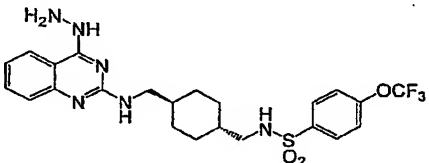
Example No.	Structure	ESI-MS	Retention Time (min)
2777	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	503.6 (M + H)	3.97
2778	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	553.8 (M + H)	4.17
2779	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(C)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	3.87
2780	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4ccc(Br)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	4.04
2781	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4cc(Cl)cc(Cl)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	537.4 (M + H)	4.23
2782	 <chem>NCCNc1nc2ccccc2n1CNC3CCCCC3NS(=O)(=O)c4cc(Br)cc(OC(F)(F)F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	631.6 (M + H)	4.23

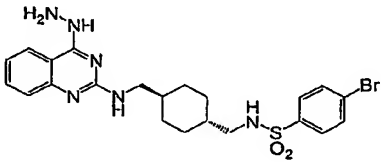
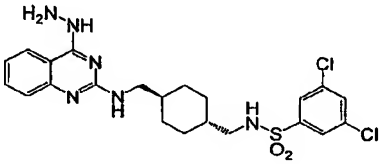
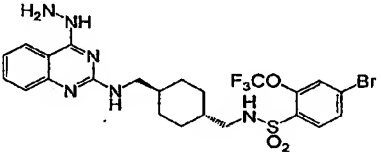
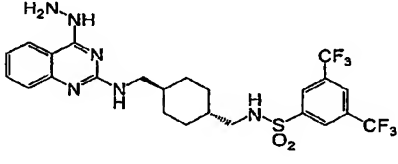
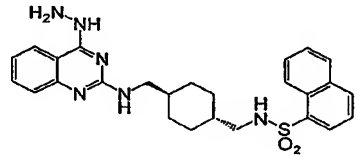
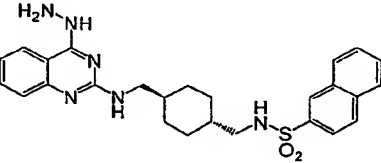
Example No.	Structure	ESI-MS	Retention Time (min)
2783	 $2\text{CF}_3\text{CO}_2\text{H}$	605.8 (M + H)	4.41
2784	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.01
2785	 $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.07
2786	 $3\text{CF}_3\text{CO}_2\text{H}$	562.6 (M + H)	3.77
2787	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	3.90
2788	 $2\text{CF}_3\text{CO}_2\text{H}$	531.6 (M + H)	4.04

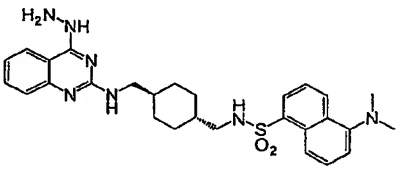
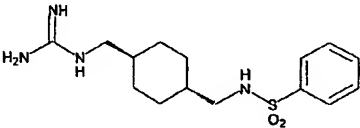
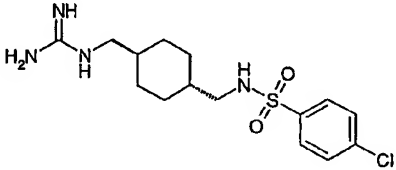
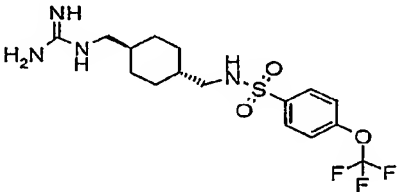
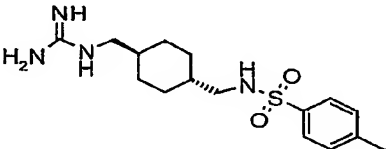
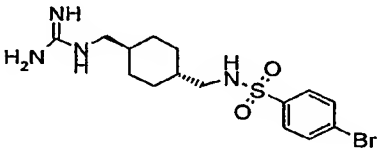
Example No.	Structure	ESI-MS	Retention Time (min)
2789	 <chem>2CF3CO2H</chem>	599.6 (M + H)	4.24
2790	 <chem>2CF3CO2H</chem>	575.0 (M + H)	3.95
2791	 <chem>2CF3CO2H</chem>	557.6 (M + H)	3.86
2792	 <chem>2CF3CO2H</chem>	565.6 (M + H)	4.03
2793	 <chem>2CF3CO2H</chem>	554 (M + H)	4.29
2794	 <chem>2CF3CO2H</chem>	503.6 (M + H)	3.78

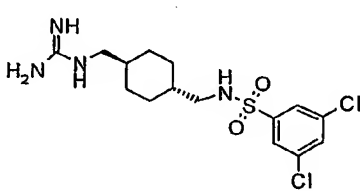
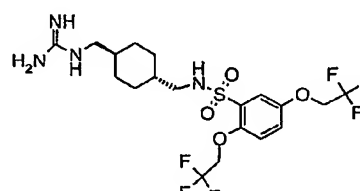
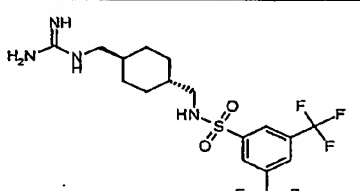
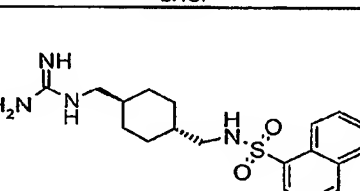
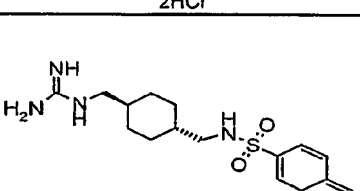
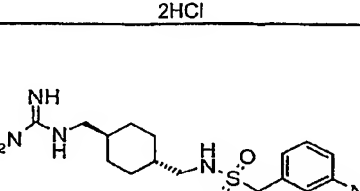
Example No.	Structure	ESI-MS	Retention Time (min)
2795	 2CF ₃ CO ₂ H	497.6 (M + H)	3.83
2796	 2CF ₃ CO ₂ H	531.6 (M + H)	4.05
2797	 2CF ₃ CO ₂ H	582.0 (M + H)	4.23
2798	 2CF ₃ CO ₂ H	511 (M + H)	3.95
2799	 2CF ₃ CO ₂ H	575.6 (M + H)	4.10
2800	 2CF ₃ CO ₂ H	565.0 (M + H)	4.32

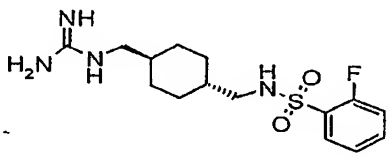
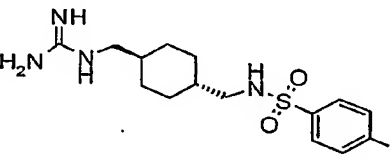
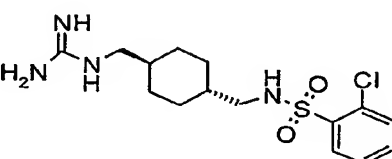
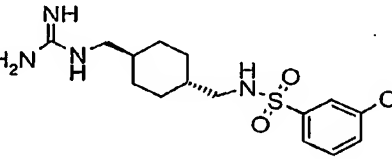
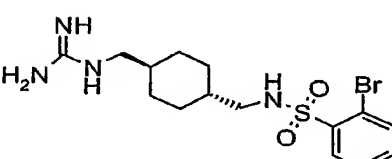
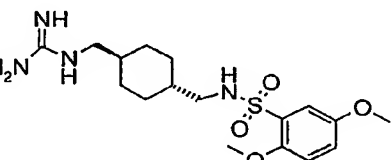
Example No.	Structure	ESI-MS	Retention Time (min)
2801	 $2\text{CF}_3\text{CO}_2\text{H}$	659.6 (M + H)	4.35
2802	 $2\text{CF}_3\text{CO}_2\text{H}$	634.0 (M + H)	4.43
2803	 $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	4.09
2804	 $2\text{CF}_3\text{CO}_2\text{H}$	547.6 (M + H)	4.15
2805	 $3\text{CF}_3\text{CO}_2\text{H}$	590.6 (M + H)	3.93
2806	 $2\text{CF}_3\text{CO}_2\text{H}$	459.6 (M + H)	4.07

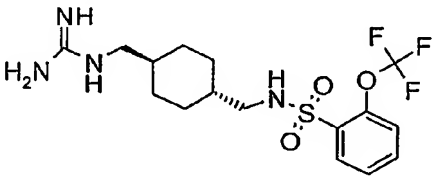
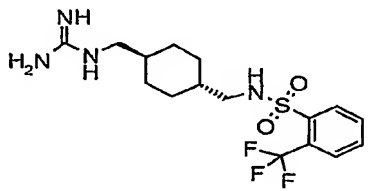
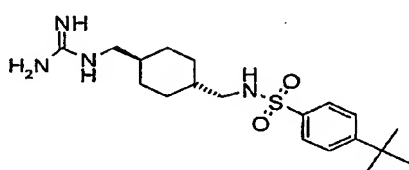
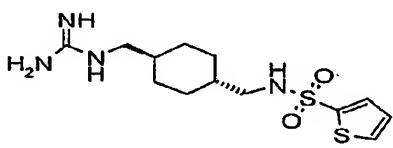
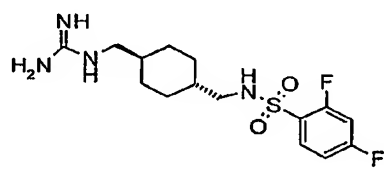
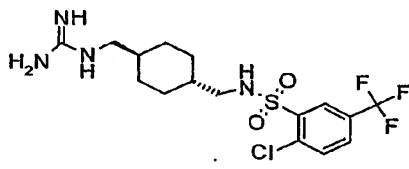
Example No.	Structure	ESI-MS	Retention Time (min)
2807	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(F)cc(F)cc3)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.6 (M + H)	4.07
2808	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3ccccc3Cl)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.07
2809	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cccc(Cl)c3)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	475.6 (M + H)	4.23
2810	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3cc(OC)cc(OC)c3)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	501.8 (M + H)	4.15
2811	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3ccccc3C(F)(F)F)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.27
2812	 <chem>Nc1nc2c(ncn2C1CCN(S(=O)(=O)c3ccc(OC(F)(F)F)cc3)CC4CCCCC4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	525.6 (M + H)	4.37

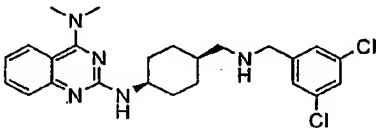
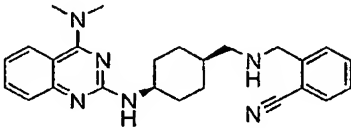
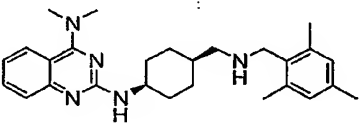
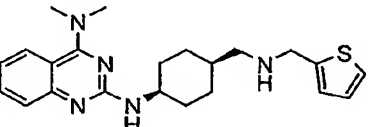
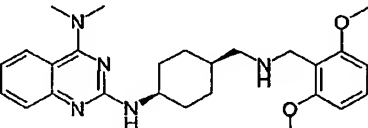
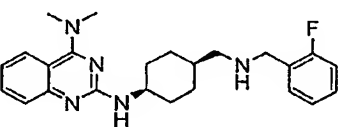
Example No.	Structure	ESI-MS	Retention Time (min)
2813	 <chem>BrC1=CC=C(S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3)C=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	519.6 (M + H)	4.25
2814	 <chem>ClC1=CC(=C(C=C1)Cl)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	509.4 (M + H)	4.49
2815	 <chem>BrC1=CC(=C(C=C1)C(F)(F)F)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	603.0 (M + H)	4.60
2816	 <chem>FC(F)(F)C1=CC(=C(C=C1)S(=O)(=O)NCC2CCCCC2CNc3nc4ccccc4n3)C(F)(F)F=C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	577.6 (M + H)	4.72
2817	 <chem>c1ccc2ccccc2c1S(=O)(=O)NCC3CCCCC3CNc4nc5ccccc5n4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491 (M + H)	4.31
2818	 <chem>c1ccc2ccccc2c1S(=O)(=O)NCC3CCCCC3CNc4nc5ccccc5n4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491.6 (M + H)	4.33

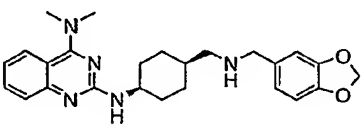
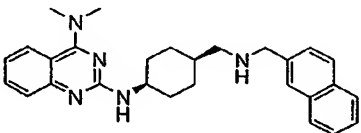
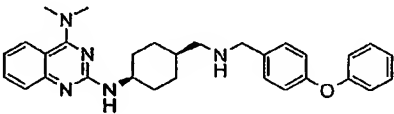
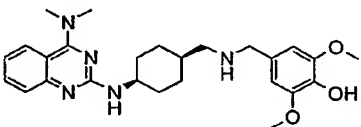
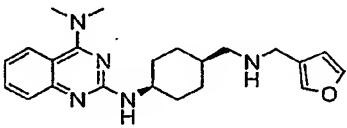
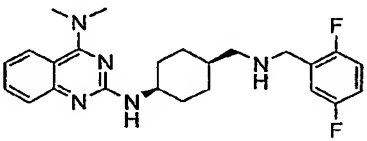
Example No.	Structure	ESI-MS	Retention Time (min)
2819	 <chem>CC1=CC=C2C(=C1)C(=CC=C2)NS(=O)(=O)CC3CCCCC3CNc4nc5ccccc5n4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	534.6 (M + H)	4.01
2820	 <chem>NS(=O)(=O)c1ccccc1CC2CCCCC2CNc3[nH]c(=N)[nH]3</chem> 2HCl	325.4 (M + H)	3.91
2821	 <chem>Clc1ccc(S(=O)(=O)NC2CCCCC2CNc3[nH]c(=N)[nH]3)cc1</chem> 2HCl	359.4 (M + H)	4.24
2822	 <chem>COc1ccc(S(=O)(=O)NC2CCCCC2CNc3[nH]c(=N)[nH]3)cc1F(F)F</chem> 2HCl	409.4 (M + H)	4.51
2823	 <chem>CC1=CC=C(S(=O)(=O)NC2CCCCC2CNc3[nH]c(=N)[nH]3)C=C1</chem> 2HCl	339.6 (M + H)	4.09
2824	 <chem>BrC1=CC=C(S(=O)(=O)NC2CCCCC2CNc3[nH]c(=N)[nH]3)C=C1</chem> 2HCl	403.4 (M + H)	4.28

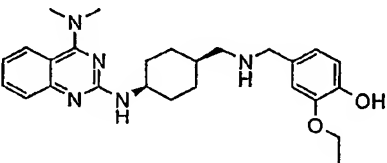
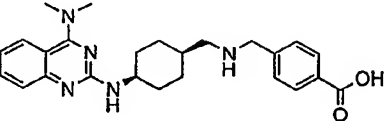
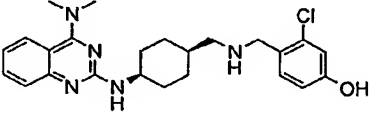
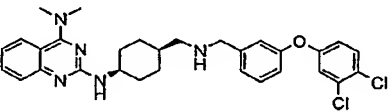
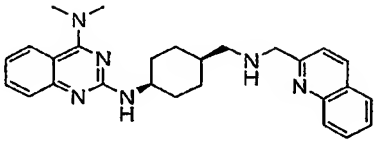
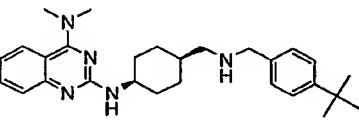
Example No.	Structure	ESI-MS	Retention Time (min)
2825	 2HCl	393.0 (M + H)	4.57
2826	 2HCl	521.6 (M + H)	4.69
2827	 2HCl	461.6 (M + H)	4.77
2828	 2HCl	375.4 (M + H)	4.33
2829	 2HCl	375.4 (M + H)	4.39
2830	 2HCl	418.8 (M + H)	4.33

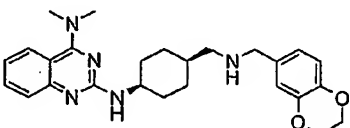
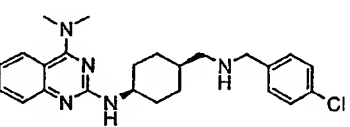
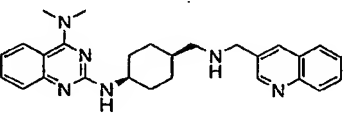
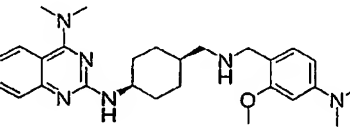
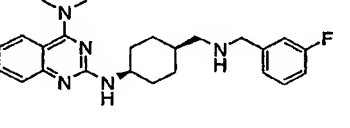
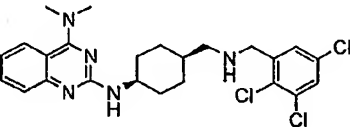
Example No.	Structure	ESI-MS	Retention Time (min)
2831	 2HCl	343.4 (M + H)	3.96
2832	 2HCl	343.4 (M + H)	4.03
2833	 2HCl	359.4 (M + H)	4.05
2834	 2HCl	359.4 (M + H)	4.24
2835	 2HCl	403.4 (M + H)	4.07
2836	 2HCl	385.4 (M + H)	4.00

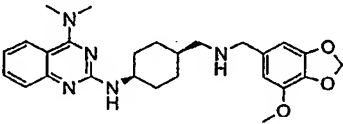
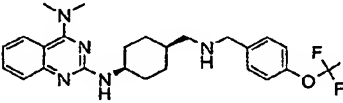
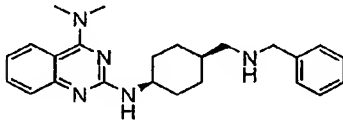
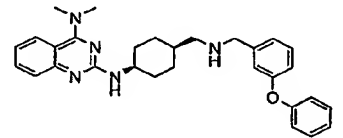
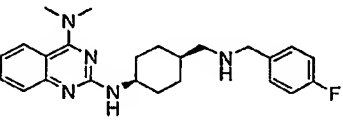
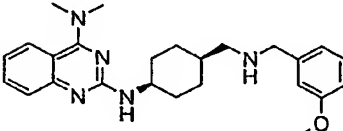
Example No.	Structure	ESI-MS	Retention Time (min)
2837	 2HCl	409.4 (M + H)	4.32
2838	 2HCl	393.6 (M + H)	4.23
2839	 2HCl	381.6 (M + H)	4.62
2840	 2HCl	330.8 (M + H)	3.83
2841	 2HCl	361.4 (M + H)	4.05
2842	 2HCl	427.4 (M + H)	4.51

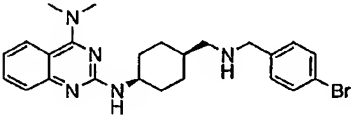
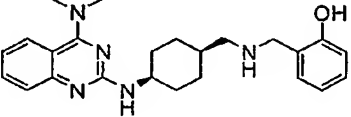
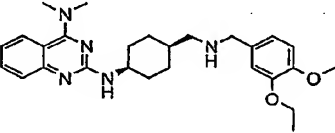
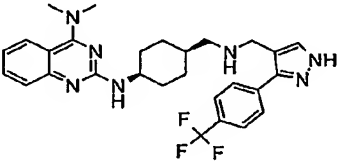
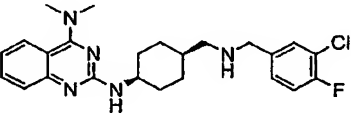
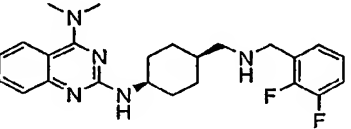
Example No.	Structure	ESI-MS	Retention Time (min)
2843	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)Cl)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.22
2844	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C5C(=C4)NCC5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	3.01
2845	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)C)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.6 (M + H)	3.26
2846	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C5C(=C4)S5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.81
2847	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)OC)OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.09
2848	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(=C(C=C4)F)</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.85

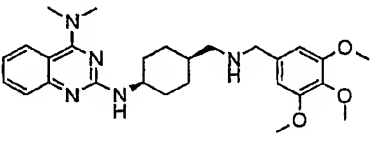
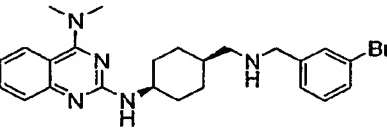
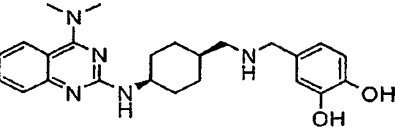
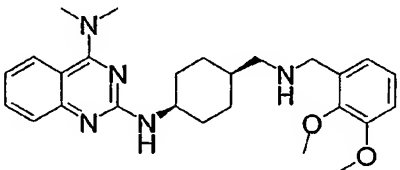
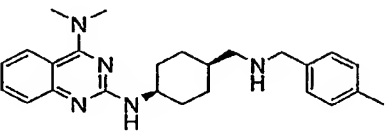
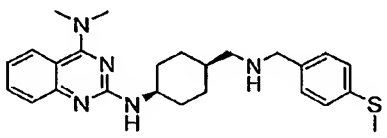
Example No.	Structure	ESI-MS	Retention Time (min)
2849	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C5C(=C4)OC5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.89
2850	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C5C=CC6=CC=CC=C456</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.20
2851	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=C(C=C4)OC(=O)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
2852	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(OC)=C(O)C=C4OC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.71
2853	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC=CC=C4O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.72
2854	 <chem>CN1C=NC2=CC=CC=C2N1C3CCCCC3NC4=CC(F)=CC(F)=C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.91

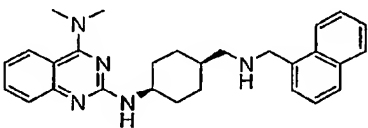
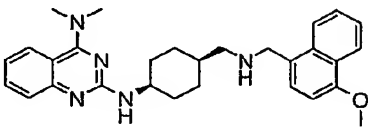
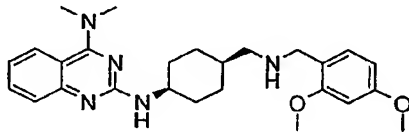
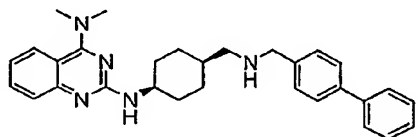
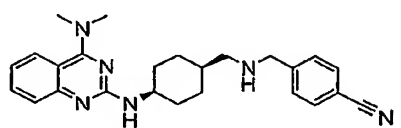
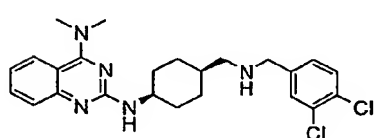
Example No.	Structure	ESI-MS	Retention Time (min)
2855	 <chem>CCOC1=CC=C(C=C1CNC2CCCCC2Nc3nc4ccccc4n3C)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.82
2856	 <chem>OC(=O)C1=CC=C(C=C1CNC2CCCCC2Nc3nc4ccccc4n3C)</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.69
2857	 <chem>ClC1=CC=C(C=C1CNC2CCCCC2Nc3nc4ccccc4n3C)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	2.85
2858	 <chem>ClC1=CC(=C(C=C1CNC2CCCCC2Nc3nc4ccccc4n3C)OC(=O)C)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	550.6 (M + H)	3.80
2859	 <chem>CN1C=NC2=C(N1)C=CC=C2C3CCCCC3NC4CCCCC4Nc5nc6ccccc6n5</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.03
2860	 <chem>CC(C)(C)C1=CC=C(C=C1CNC2CCCCC2Nc3nc4ccccc4n3C)</chem> $2\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	3.41

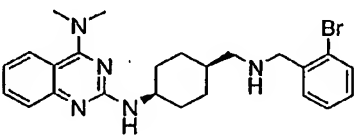
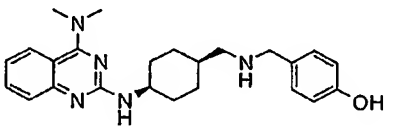
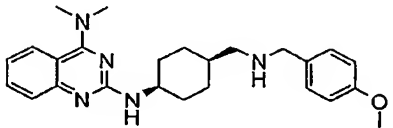
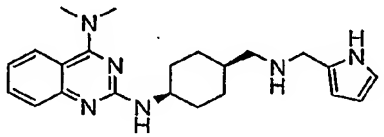
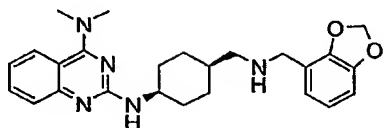
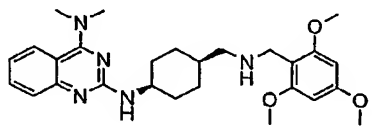
Example No.	Structure	ESI-MS	Retention Time (min)
2861	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5cc6ccccc5O6)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.91
2862	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5ccc(Cl)cc5)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.05
2863	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5cnc6ccccc56)c2</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.68
2864	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5cc(OC)cc(N(C)C)c5)c2</chem> $3\text{CF}_3\text{CO}_2\text{H}$	463.4 (M + H)	2.76
2865	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5ccc(F)cc5)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2866	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4CNc5cc(Cl)c(Cl)cc5)c2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.30

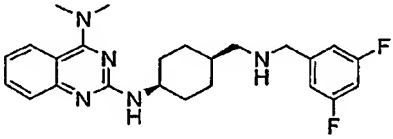
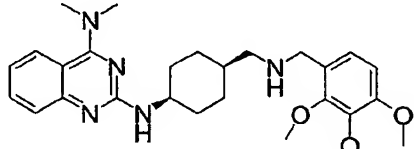
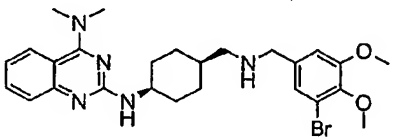
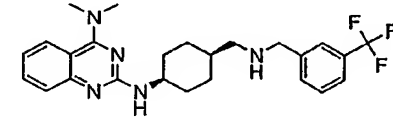
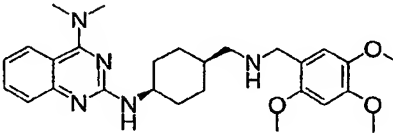
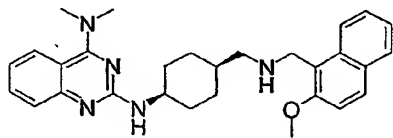
Example No.	Structure	ESI-MS	Retention Time (min)
2867	 <chem>COc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.93
2868	 <chem>COc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.27
2869	 <chem>c1ccccc1CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.6 (M + H)	2.88
2870	 <chem>c1ccc(cc1)Oc2ccc(cc2)CNCC3CCCCC3Nc4nc5ccccc5n4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.43
2871	 <chem>Fc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	2.91
2872	 <chem>COc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.91

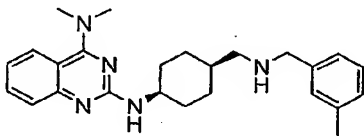
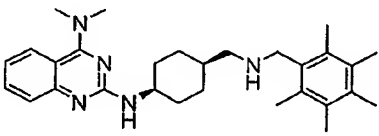
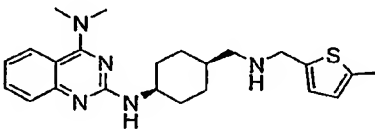
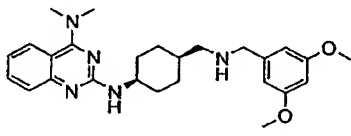
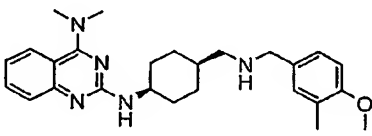
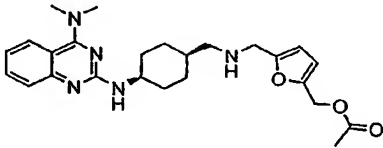
Example No.	Structure	ESI-MS	Retention Time (min)
2873	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(Br)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.09
2874	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(O)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
2875	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(OC)c(OC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	2.97
2876	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4ccc(C(F)(F)F)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.12
2877	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)c(Cl)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	3.10
2878	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CNc4cc(F)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.90

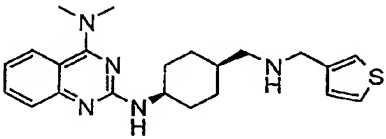
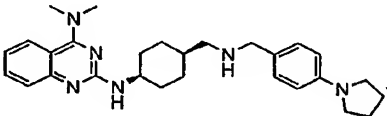
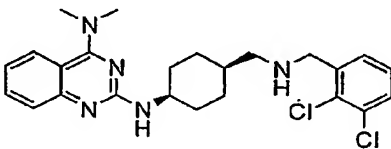
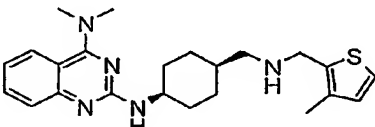
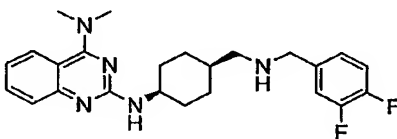
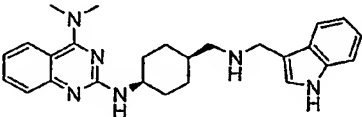
Example No.	Structure	ESI-MS	Retention Time (min)
2879	 <chem>COc1ccc(cc1)CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.89
2880	 <chem>BrC1=CC=C(C=C1)CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.07
2881	 <chem>Oc1cc(O)ccc1CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.4 (M + H)	2.61
2882	 <chem>COc1cc(OC)ccc1CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	2.93
2883	 <chem>Cc1ccc(cc1)CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	404.6 (M + H)	3.01
2884	 <chem>Ic1ccc(cc1)CNCC2(CCC(C)CC2)CNc3nc4c(ncn3C)ccccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.08

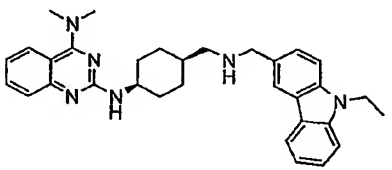
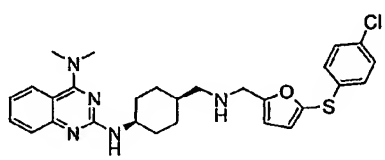
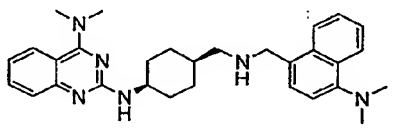
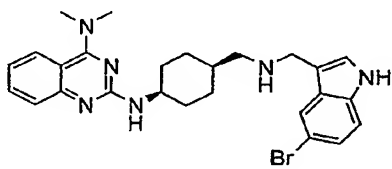
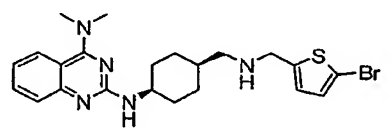
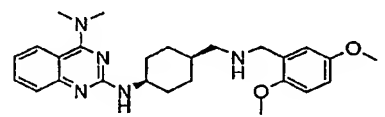
Example No.	Structure	ESI-MS	Retention Time (min)
2885	 <chem>CN(C)c1nc2c(ncn2C1CCNCCc3ccccc3)cccc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.18
2886	 <chem>COc1ccccc1CNCCc2ccccc2N1C=NC2=CC=CC=C2N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.25
2887	 <chem>COc1cc(OC)ccc1CNCCc2ccccc2N1C=NC2=CC=CC=C2N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.01
2888	 <chem>c1ccc(cc1)CNCCc2ccccc2N1C=NC2=CC=CC=C2N1C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.40
2889	 <chem>N#Cc1ccc(CNCCc2ccccc2N1C=NC2=CC=CC=C2N1C)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.83
2890	 <chem>Clc1cc(CNCCc2ccccc2N1C=NC2=CC=CC=C2N1C)cc(Cl)c1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.25

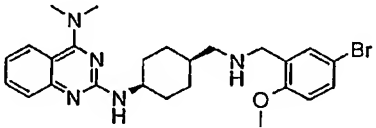
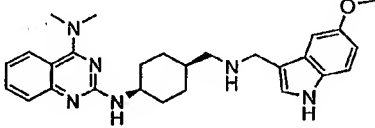
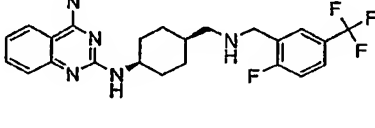
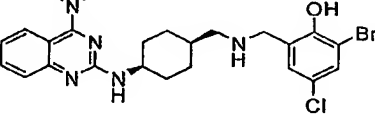
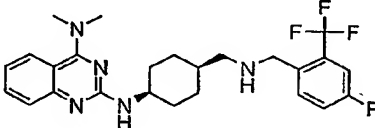
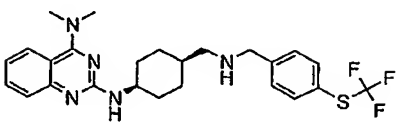
Example No.	Structure	ESI-MS	Retention Time (min)
2891	 $2\text{CF}_3\text{CO}_2\text{H}$	468.2 (M + H)	3.00
2892	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.66
2893	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.92
2894	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.71
2895	 $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	2.87
2896	 $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.17

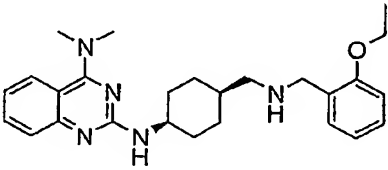
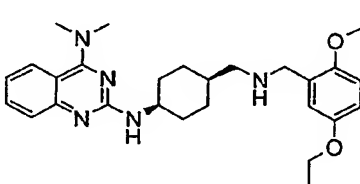
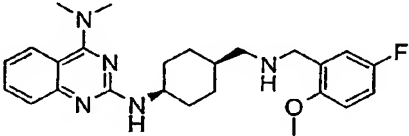
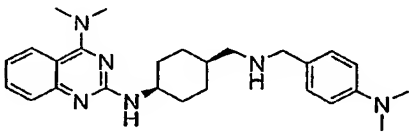
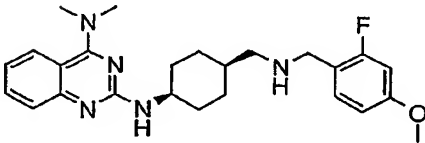
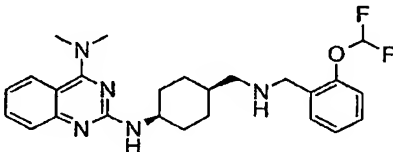
Example No.	Structure	ESI-MS	Retention Time (min)
2897	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4ccc(F)c(F)c4)Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.98
2898	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(OC)c(OC)c(OC)c4)Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.99
2899	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(OC)c(Br)c(OC)c4)Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.4 (M + H)	3.15
2900	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4ccc(C(F)(F)F)cc4)Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.19
2901	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4cc(OC)c(OC)c(OC)c4)Cc5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.92
2902	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CN[C@@H](Cc4c5ccccc5c(OC)c4)Cc6ccccc6</chem> $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	3.27

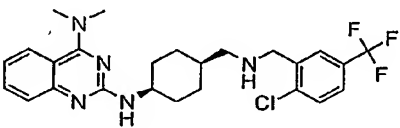
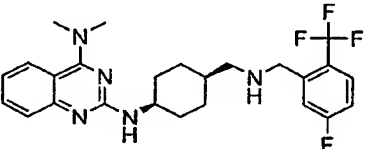
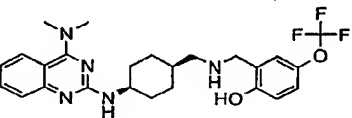
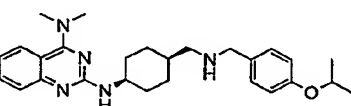
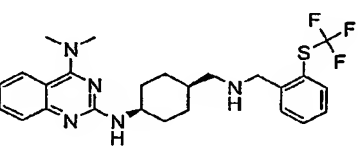
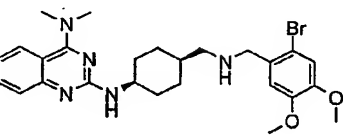
Example No.	Structure	ESI-MS	Retention Time (min)
2903	 2CF ₃ CO ₂ H	404.6 (M + H)	2.87
2904	 2CF ₃ CO ₂ H	460.4 (M + H)	3.48
2905	 2CF ₃ CO ₂ H	410.4 (M + H)	2.96
2906	 2CF ₃ CO ₂ H	450.0 (M + H)	3.03
2907	 2CF ₃ CO ₂ H	434.4 (M + H)	3.08
2908	 2CF ₃ CO ₂ H	452.2 (M + H)	2.79

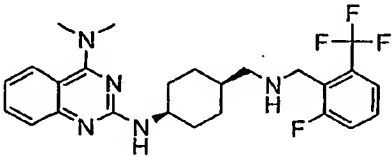
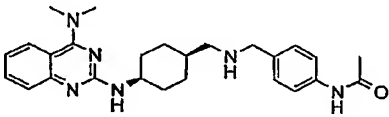
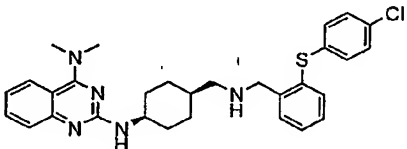
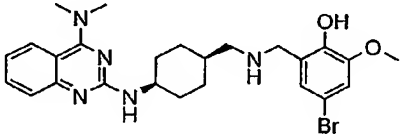
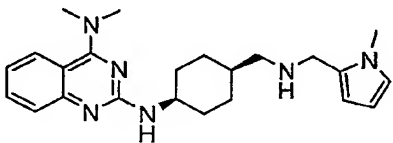
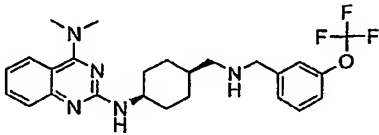
Example No.	Structure	ESI-MS	Retention Time (min)
2909	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.81
2910	 $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	3.21
2911	 $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.08
2912	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.88
2913	 $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.01
2914	 $3\text{CF}_3\text{CO}_2\text{H}$	429.4 (M + H)	2.97

Example No.	Structure	ESI-MS	Retention Time (min)
2915	 $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.53
2916	 $2\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	3.56
2917	 $3\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.80
2918	 $3\text{CF}_3\text{CO}_2\text{H}$	507.2 (M + H)	3.27
2919	 $2\text{CF}_3\text{CO}_2\text{H}$	474.2 (M + H)	3.10
2920	 $2\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.00

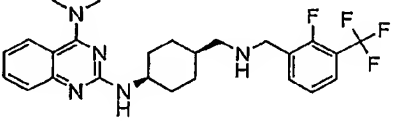
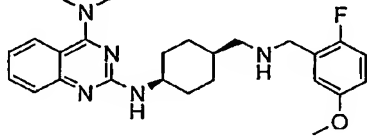
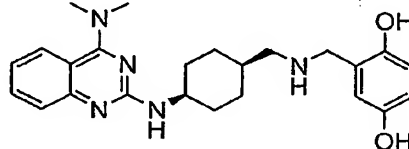
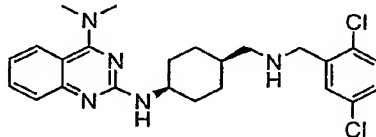
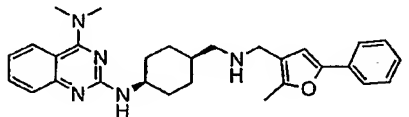
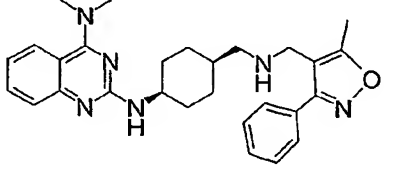
Example No.	Structure	ESI-MS	Retention Time (min)
2921	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)OC)C5=CC=CC=C5Br</chem> $2\text{CF}_3\text{CO}_2\text{H}$	498.4 (M + H)	3.15
2922	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4C=CC(OC)C=C4)C5=CC=CC=C5</chem> $3\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	2.99
2923	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)F)C5=CC=C(C=C5)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.0 (M + H)	3.10
2924	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)O)C5=CC(=C(C=C5)Br)Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	518.2 (M + H)	3.10
2925	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)F)C5=CC(=C(C=C5)F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.12
2926	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC4=CC=C(C=C4)SC(F)(F)F)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35

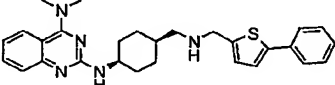
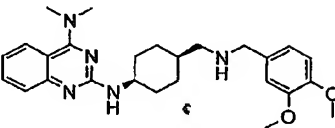
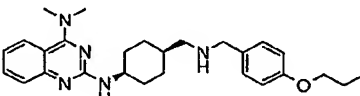
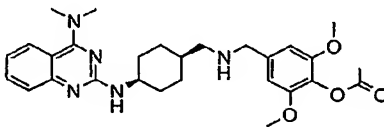
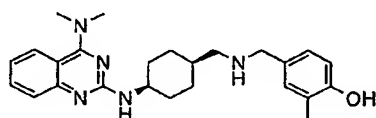
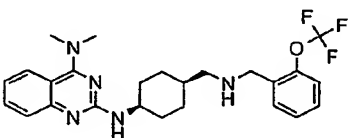
Exemplé No.	Structure	ESI-MS	Retention Time (min)
2927	 2CF ₃ CO ₂ H	434.4 (M + H)	3.11
2928	 2CF ₃ CO ₂ H	478.4 (M + H)	3.29
2929	 2CF ₃ CO ₂ H	438.2 (M + H)	3.01
2930	 3CF ₃ CO ₂ H	433.4 (M + H)	2.59
2931	 2CF ₃ CO ₂ H	438.2 (M + H)	2.90
2932	 2CF ₃ CO ₂ H	456.2 (M + H)	3.10

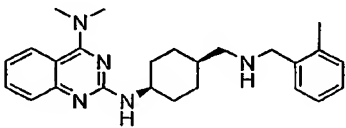
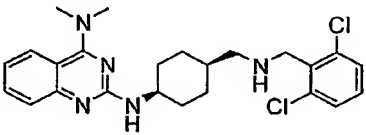
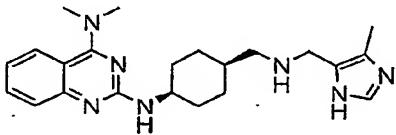
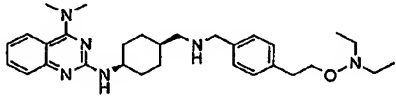
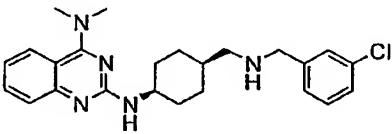
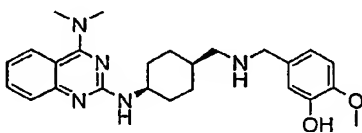
Example No.	Structure	ESI-MS	Retention Time (min)
2933	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCC4=CC=C(C(F)(F)F)C=C4Cl)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.2 (M + H)	3.25
2934	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCC4=CC=C(C(F)(F)F)C=C4F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.11
2935	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCC4=CC=C(OC(F)(F)F)C=C4O)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.20
2936	 <chem>CC(C)Oc1ccc(cc1NCC2CCCCC2NCC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C54)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.17
2937	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCC4=CC=C(C(F)(F)F)C=C4)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	489.6 (M + H)	3.31
2938	 <chem>COc1cc(OC)c(Br)cc1NCC2CCCCC2NCC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C54</chem> $2\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	3.03

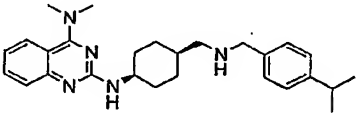
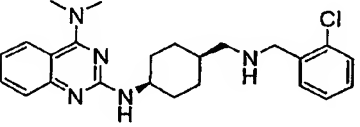
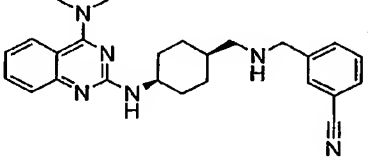
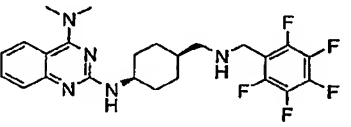
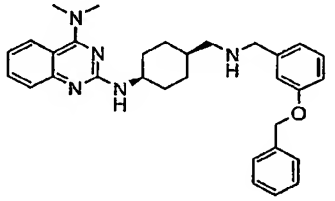
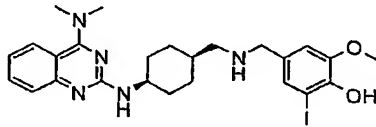
Example No.	Structure	ESI-MS	Retention Time (min)
2939	 2CF ₃ CO ₂ H	476.2 (M + H)	2.99
2940	 2CF ₃ CO ₂ H	447.4 (M + H)	2.66
2941	 2CF ₃ CO ₂ H	532.4 (M + H)	3.66
2942	 2CF ₃ CO ₂ H	514.4 (M + H)	3.08
2943	 3CF ₃ CO ₂ H	393.4 (M + H)	2.79
2944	 2CF ₃ CO ₂ H	474.4 (M + H)	3.24

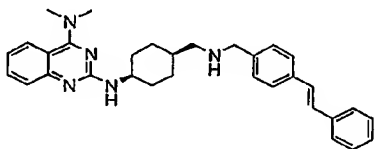
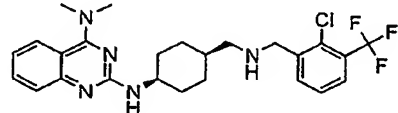
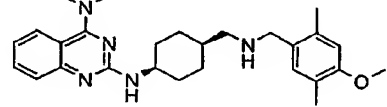
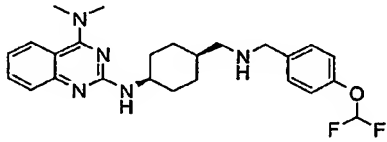
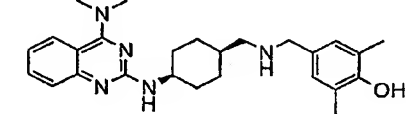
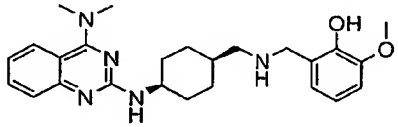
Example No.	Structure	ESI-MS	Retention Time (min)
2945	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C(F)(F)F)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.44
2946	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C(F)(F)F)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	3.42
2947	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C(F)(F)F)cc(S)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.35
2948	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4ccc(OCC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.43
2949	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C)cc(C)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.13
2950	 <chem>CN(C)c1nc2c(ncn2C1)N[C@H]3CCCC[C@H]3CNCCc4cc(C(F)(F)F)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.10

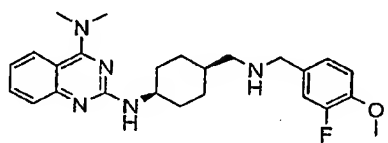
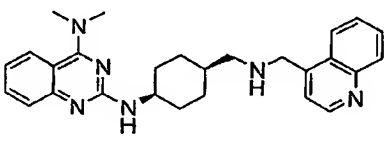
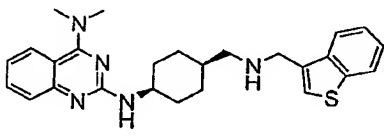
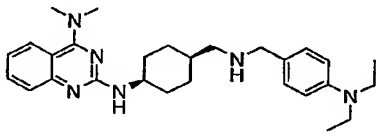
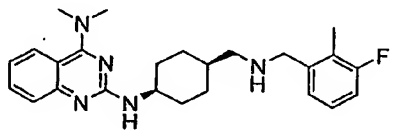
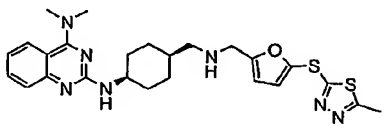
Example No.	Structure	ESI-MS	Retention Time (min)
2951	 2CF ₃ CO ₂ H	476.4 (M + H)	3.19
2952	 2CF ₃ CO ₂ H	438.2 (M + H)	2.95
2953	 2CF ₃ CO ₂ H	422.4 (M + H)	2.61
2954	 2CF ₃ CO ₂ H	458.2 (M + H)	3.07
2955	 2CF ₃ CO ₂ H	470.4 (M + H)	3.45
2956	 2CF ₃ CO ₂ H	471.6 (M + H)	2.88

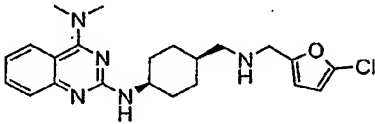
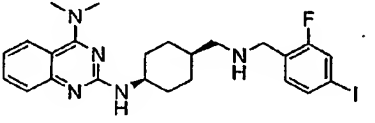
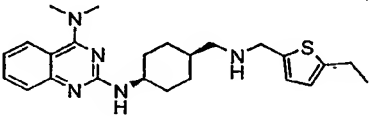
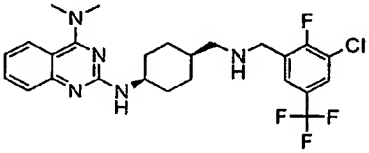
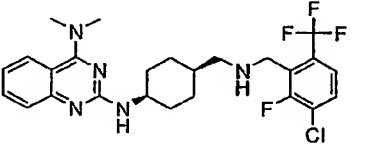
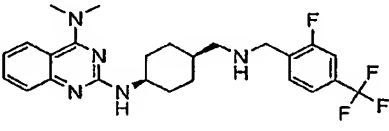
Example No.	Structure	ESI-MS	Retention Time (min)
2957	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4cc5ccccc5s4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.36
2958	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4ccc(OC)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450 (M + H)	2.75
2959	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4ccc(OCC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.20
2960	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4c(OC)c(OC(=O)C)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	508.4 (M + H)	3.00
2961	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4ccc(O)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.80
2962	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3CCc4ccc(OC(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.20

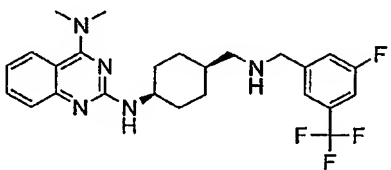
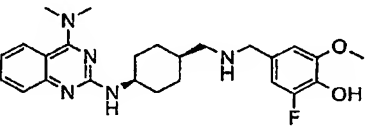
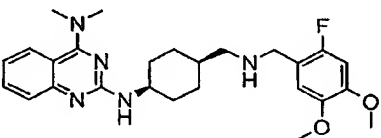
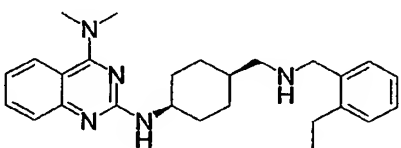
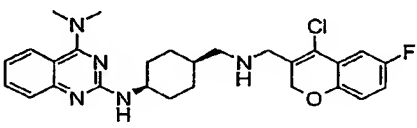
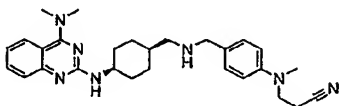
Example No.	Structure	ESI-MS	Retention Time (min)
2963	 $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	2.87
2964	 $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.00
2965	 $3\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.30
2966	 $2\text{CF}_3\text{CO}_2\text{H}$	505.4 (M + H)	2.60
2967	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.00
2968	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.71

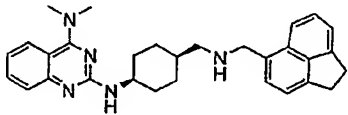
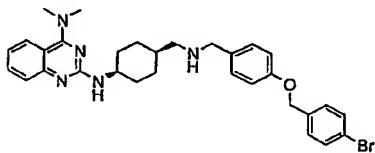
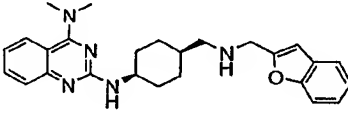
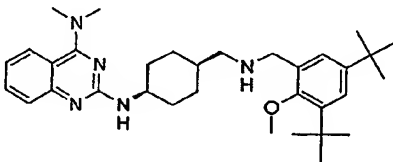
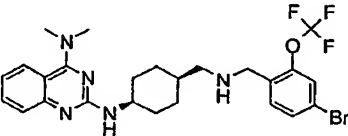
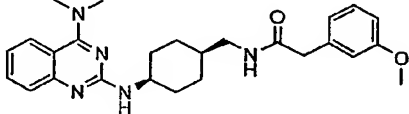
Example No.	Structure	ESI-MS	Retention Time (min)
2969	 <chem>CC(C)c1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.30
2970	 <chem>Clc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.95
2971	 <chem>N#Cc1ccc(cc1)CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	2.79
2972	 <chem>Fc1cc(F)c(F)c(F)c1CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.00
2973	 <chem>c1ccc(cc1)Oc2ccc(cc2)CNCC3CCCCC3Nc4nc5ccccc5n4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.2 (M + H)	3.46
2974	 <chem>COc1cc(O)ccc1CNCC2CCCCC2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	562.2 (M + H)	2.99

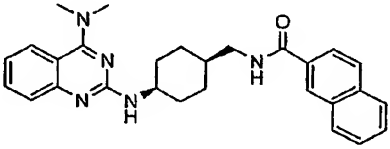
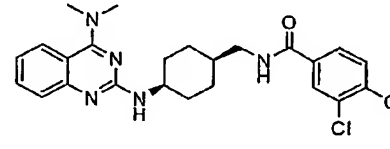
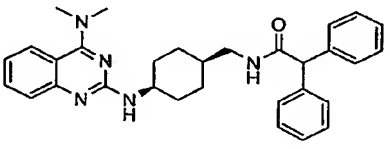
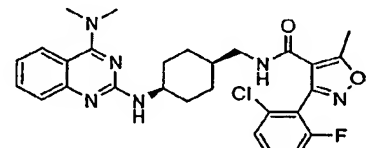
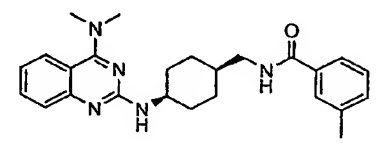
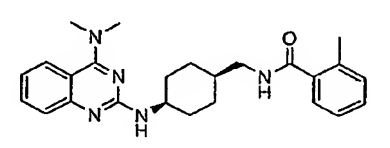
Example No.	Structure	ESI-MS	Retention Time (min)
2975	 2CF ₃ CO ₂ H	492.4 (M + H)	3.64
2976	 2CF ₃ CO ₂ H	492.2 (M + H)	3.25
2977	 2CF ₃ CO ₂ H	448.4 (M + H)	3.22
2978	 2CF ₃ CO ₂ H	456.2 (M + H)	3.09
2979	 2CF ₃ CO ₂ H	434.4 (M + H)	2.89
2980	 2CF ₃ CO ₂ H	436.4 (M + H)	2.79

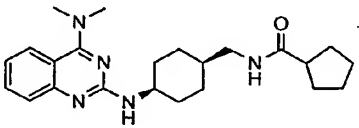
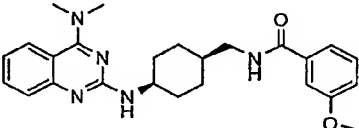
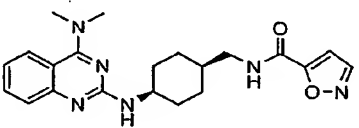
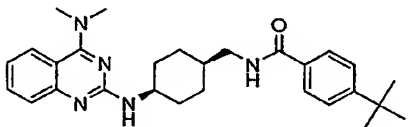
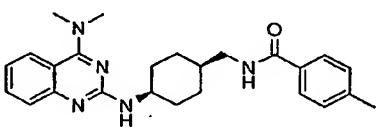
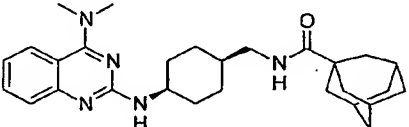
Example No.	Structure	ESI-MS	Retention Time (min)
2981	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4ccc(OC)c(F)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	2.91
2982	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4cnc5ccccc45</chem> $3\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	2.55
2983	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4c5ccccc4s5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	446.4 (M + H)	3.13
2984	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4ccc(NCC)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	461.4 (M + H)	2.46
2985	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4ccccc4F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.01
2986	 <chem>CN(C)c1nc2ccccc2n1NC3CCCCC3NCc4oc5nn(s45)C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	510.2 (M + H)	2.85

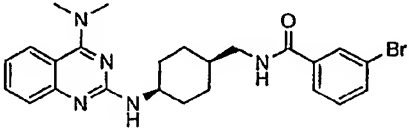
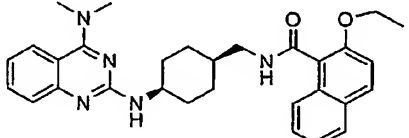
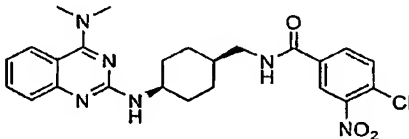
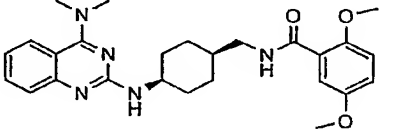
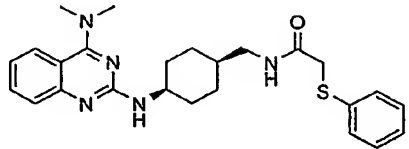
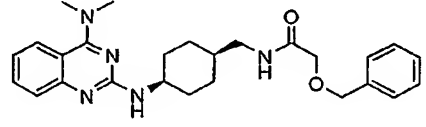
Example No.	Structure	ESI-MS	Retention Time (min)
2987	 $2\text{CF}_3\text{CO}_2\text{H}$	414.4 (M + H)	2.86
2988	 $2\text{CF}_3\text{CO}_2\text{H}$	534.2 (M + H)	3.13
2989	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.08
2990	 $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.32
2991	 $2\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
2992	 $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.17

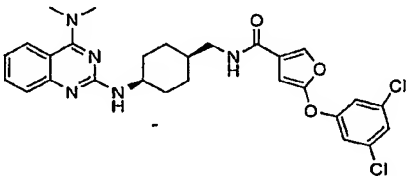
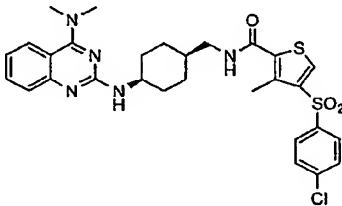
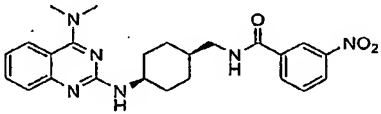
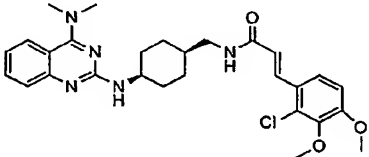
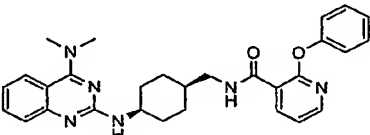
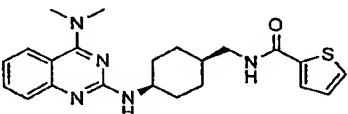
Example No.	Structure	ESI-MS	Retention Time (min)
2993	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4cc(F)c(C(F)(F)F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.21
2994	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(F)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.77
2995	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4cc(OC)c(F)c(OC)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.89
2996	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4ccccc4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.12
2997	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4cc5c(cc4)oc6cc(F)ccc6Cl5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
2998	 <chem>CC1=NC2=C(N1)N=CN=C2N[C@H]3CCCC[C@H]3CNCCc4ccc(N(C)C#N)cc4</chem> $3\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	2.99

Example No.	Structure	ESI-MS	Retention Time (min)
2999	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.37
3000	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	574.2 (M + H)	3.64
3001	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	430.4 (M + H)	3.05
3002	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	4.05
3003	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.37
3004	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC4=CC=CC=C4N3)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.51

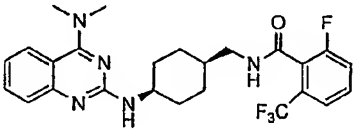
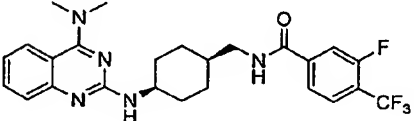
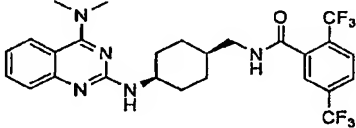
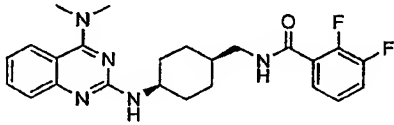
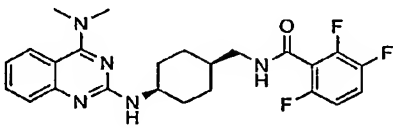
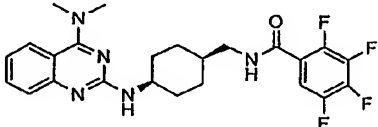
Example No.	Structure	ESI-MS	Retention Time (min)
3005	 CF ₃ CO ₂ H	454.2 (M + H)	3.91
3006	 CF ₃ CO ₂ H	472.4 (M + H)	4.02
3007	 CF ₃ CO ₂ H	494.4 (M + H)	4.01
3008	 CF ₃ CO ₂ H	537.4 (M + H)	3.77
3009	 CF ₃ CO ₂ H	418.6 (M + H)	3.63
3010	 CF ₃ CO ₂ H	418.6 (M + H)	3.51

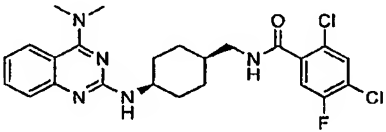
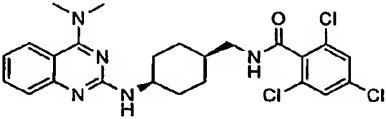
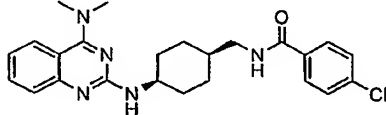
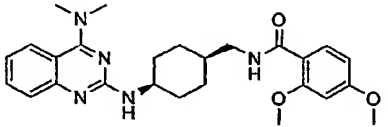
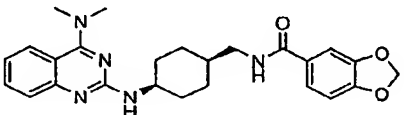
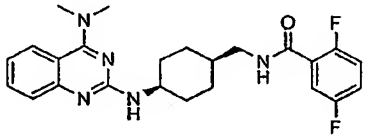
Example No.	Structure	ESI-MS	Retention Time (min)
3011	 CF ₃ CO ₂ H	396.2 (M + H)	3.47
3012	 CF ₃ CO ₂ H	434.4 (M + H)	3.52
3013	 CF ₃ CO ₂ H	395.4 (M + H)	3.15
3014	 CF ₃ CO ₂ H	460.2 (M + H)	4.03
3015	 CF ₃ CO ₂ H	418.6 (M + H)	3.65
3016	 CF ₃ CO ₂ H	462.2 (M + H)	4.09

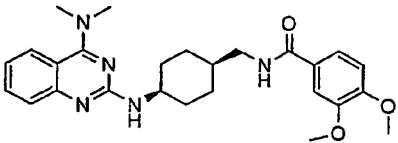
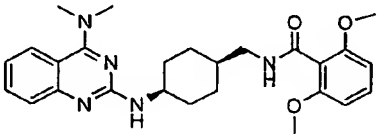
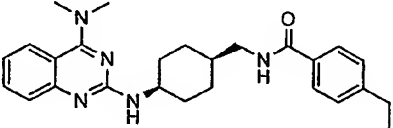
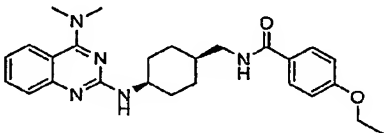
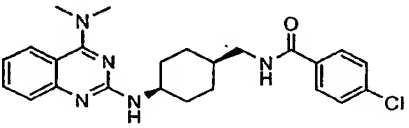
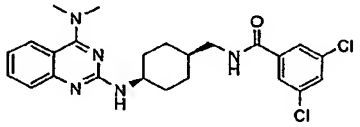
Example No.	Structure	ESI-MS	Retention Time (min)
3017	 <chem>CN1C=NC2=C(N1)C=CC=C2[C@H]3CCCC[C@H]3NC(=O)c4ccc(Br)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	3.79
3018	 <chem>CCOC1=CC=C2C(=C1)C(=O)N[C@H]3CCCC[C@H]3NC4=NC5=CC=CC=C5N(C)N4C2</chem> $\text{CF}_3\text{CO}_2\text{H}$	498.6 (M + H)	3.88
3019	 <chem>CN1C=NC2=C(N1)C=CC=C2[C@H]3CCCC[C@H]3NC(=O)c4cc([N+](=O)[O-])cc(Cl)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	3.80
3020	 <chem>COC1=CC(OC)=C(C(=O)N[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)N3)C=C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.49
3021	 <chem>CN1C=NC2=C(N1)C=CC=C2[C@H]3CCCC[C@H]3NC(=O)CCSC4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.0 (M + H)	3.61
3022	 <chem>CN1C=NC2=C(N1)C=CC=C2[C@H]3CCCC[C@H]3NC(=O)COCC4=CC=CC=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.2 (M + H)	3.70

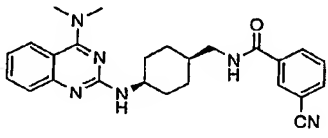
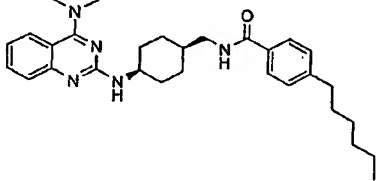
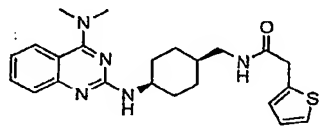
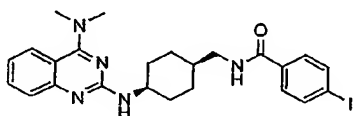
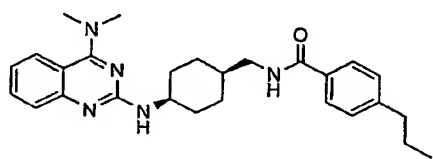
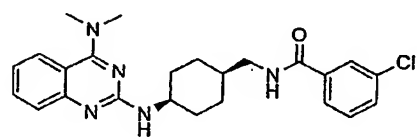
Example No.	Structure	ESI-MS	Retention Time (min)
3023	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	554.4 (M + H)	4.41
3024	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	598.2 (M + H)	4.03
3025	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	499.2 (M + H)	3.59
3026	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	524.6 (M + H)	3.84
3027	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	3.80
3028	 <chem>CC1=CC=C(C=C1)C(=O)NCC2(CCC(C)CC2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.43

Example No.	Structure	ESI-MS	Retention Time (min)
3029	<p>CF₃CO₂H</p>	468.2 (M + H)	3.77
3030	<p>CF₃CO₂H</p>	463.2 (M + H)	3.73
3031	<p>CF₃CO₂H</p>	490.4 (M + H)	3.91
3032	<p>CF₃CO₂H</p>	490.4 (M + H)	3.94
3033	<p>CF₃CO₂H</p>	490.4 (M + H)	3.85
3034	<p>CF₃CO₂H</p>	490.4 (M + H)	3.87

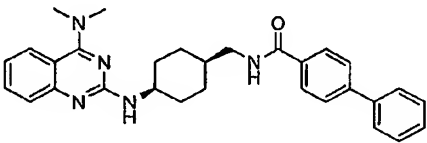
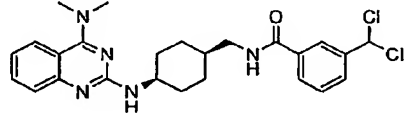
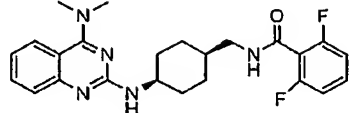
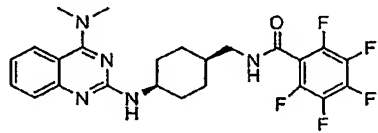
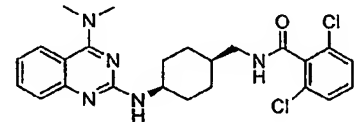
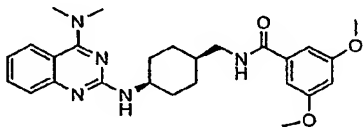
Example No.	Structure	ESI-MS	Retention Time (min)
3035	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.63
3036	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(C(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.54
3037	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	3.95
3038	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.58
3039	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.56
3040	 <chem>CC1=NC2=CC=CC=C2N(C)=CN1C3=CC=CC=C3N3CCCCC3CCNC(=O)c4cc(F)c(F)c(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.83

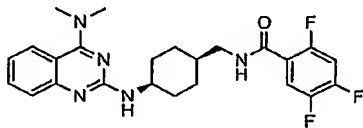
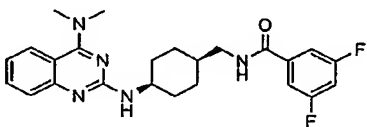
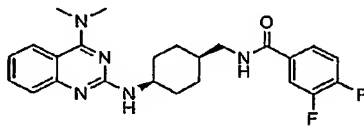
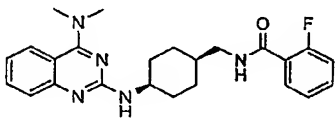
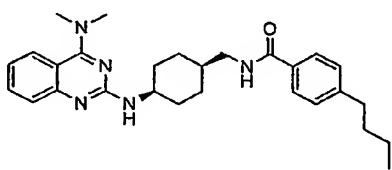
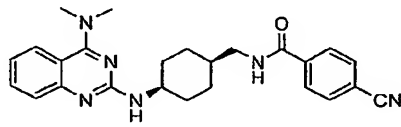
Example No.	Structure	ESI-MS	Retention Time (min)
3041	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1=NC3=CC=CC=C3N3C(=O)N(C3)C4=CC=C(C=C4)C(F)=CC(=C4)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.4 (M + H)	3.82
3042	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1=NC3=CC=CC=C3N3C(=O)N(C3)C4=CC=C(C=C4)C(=C(C=C4)Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.0 (M + H)	3.85
3043	 <chem>CC1=NC2=CC=CC=C2N(C)=NC1=NC3=CC=CC=C3N3C(=O)N(C3)C4=CC=C(C=C4)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.71
3044	 <chem>COc1cc(OC)ccc1C(=O)N(C2=CC=CC=C2N3C(=O)N(C3)C4=CC=C(C=C4)C(=C(C=C4)Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.65
3045	 <chem>COc1cc2c(c1)OCO2C(=O)N(C3=CC=CC=C3N4C(=O)N(C4)C5=CC=C(C=C5)C(=C(C=C5)Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.47
3046	 <chem>FC1=CC=C(C=C1)C(=O)N(C2=CC=CC=C2N3C(=O)N(C3)C4=CC=C(C=C4)C(=C(C=C4)Cl)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.59

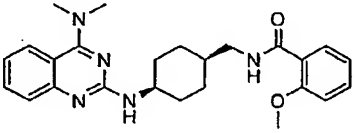
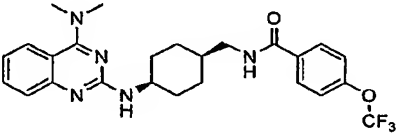
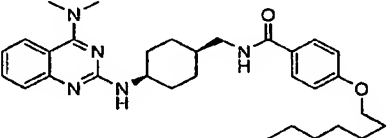
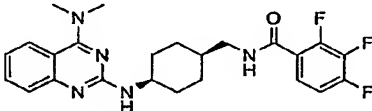
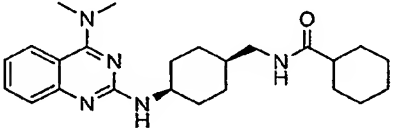
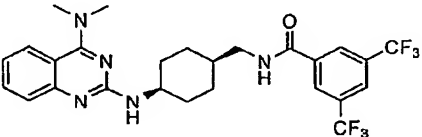
Example No.	Structure	ESI-MS	Retention Time (min)
3047	 <chem>COc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.36
3048	 <chem>COc1cc(OC)c(cc1)C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.39
3049	 <chem>CCc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.81
3050	 <chem>CCOC1=CC=C(C=C1)C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	3.69
3051	 <chem>Clc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.69
3052	 <chem>Clc1cc(Cl)ccc1C(=O)NCC2CCCCC2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	4.03

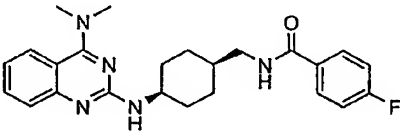
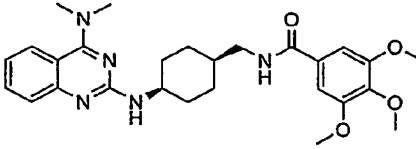
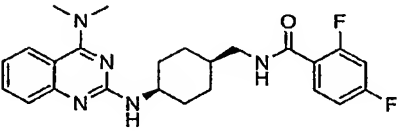
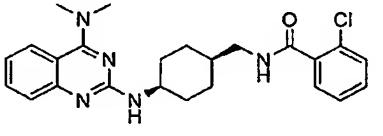
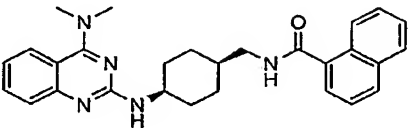
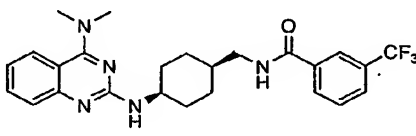
Example No.	Structure	ESI-MS	Retention Time (min)
3053	 CF ₃ CO ₂ H	429.2 (M + H)	3.47
3054	 CF ₃ CO ₂ H	488.4 (M + H)	4.60
3055	 CF ₃ CO ₂ H	424.2 (M + H)	3.41
3056	 CF ₃ CO ₂ H	530.2 (M + H)	3.83
3057	 CF ₃ CO ₂ H	446.4 (M + H)	4.02
3058	 CF ₃ CO ₂ H	438.2 (M + H)	3.70

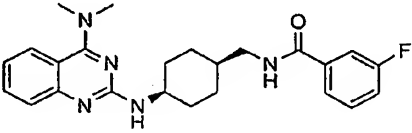
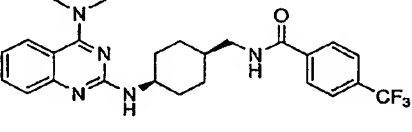
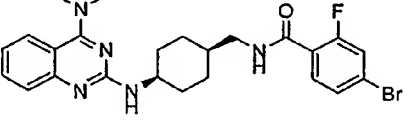
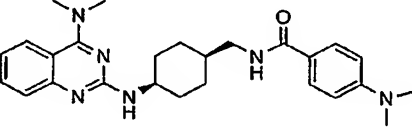
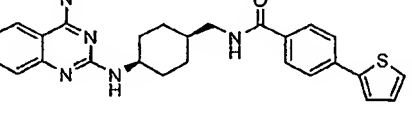
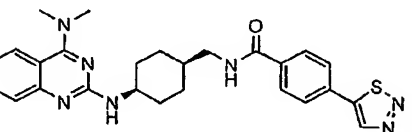
Example No.	Structure	ESI-MS	Retention Time (min)
3059	<p>CF₃CO₂H</p>	472.4 (M + H)	3.55
3060	<p>CF₃CO₂H</p>	506.4 (M + H)	3.71
3061	<p>CF₃CO₂H</p>	530.2 (M + H)	3.61
3062	<p>CF₃CO₂H</p>	474.4 (M + H)	4.41
3063	<p>CF₃CO₂H</p>	476.4 (M + H)	4.14
3064	<p>CF₃CO₂H</p>	502.4 (M + H)	4.83

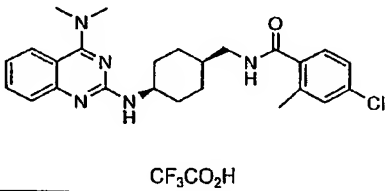
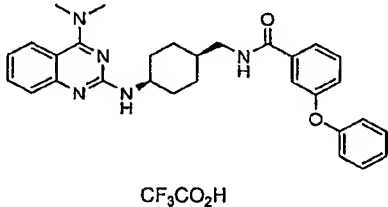
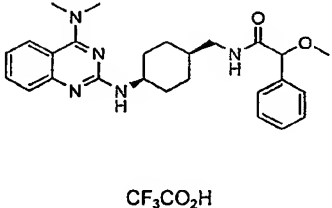
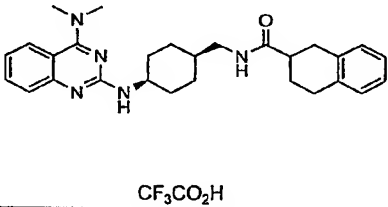
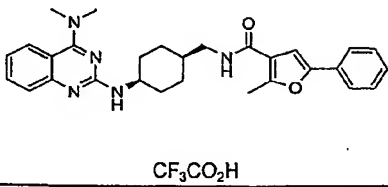
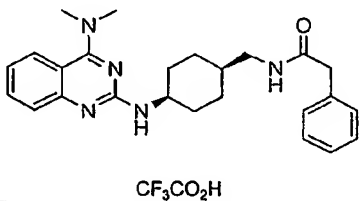
Example No.	Structure	ESI-MS	Retention Time (min)
3065	 <chem>CC1=NC2=CC=CC=C2N(C)N1C(=N)N[C@H]3CCCC[C@H]3NC(=O)C4=CC=C(C=C4)C5=CC=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.09
3066	 <chem>ClC1=CC=C(C=C1C(=O)N[C@H]2CCCC[C@H]2NC(=N)N3C=NC4=CC=CC=C4N(C)N3C=C4)C=C1Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	486.4 (M + H)	3.84
3067	 <chem>Fc1cc(F)c(NC(=O)N[C@H]2CCCC[C@H]2NC(=N)N3C=NC4=CC=CC=C4N(C)N3C=C4)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	3.46
3068	 <chem>Fc1cc(F)c(NC(=O)N[C@H]2CCCC[C@H]2NC(=N)N3C=NC4=CC=CC=C4N(C)N3C=C4)c(F)c1F</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.79
3069	 <chem>Clc1cc(NC(=O)N[C@H]2CCCC[C@H]2NC(=N)N3C=NC4=CC=CC=C4N(C)N3C=C4)c(Cl)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.55
3070	 <chem>COc1cc(NC(=O)N[C@H]2CCCC[C@H]2NC(=N)N3C=NC4=CC=CC=C4N(C)N3C=C4)c(OC)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.63

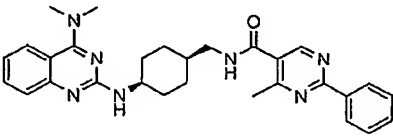
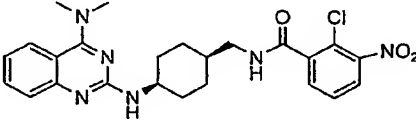
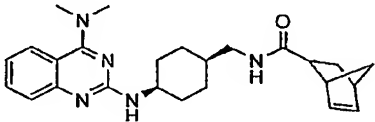
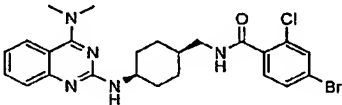
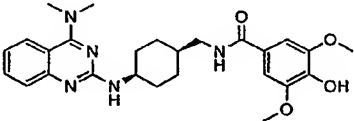
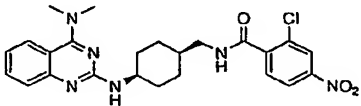
Example.No.	Structure	ESI-MS	Retention Time (min)
3071	 CF ₃ CO ₂ H	458.2 (M + H)	3.69
3072	 CF ₃ CO ₂ H	440.4 (M + H)	3.69
3073	 CF ₃ CO ₂ H	440.4 (M + H)	3.66
3074	 CF ₃ CO ₂ H	422.4 (M + H)	3.55
3075	 CF ₃ CO ₂ H	460.4 (M + H)	4.24
3076	 CF ₃ CO ₂ H	429.2 (M + H)	3.42

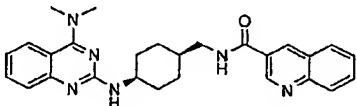
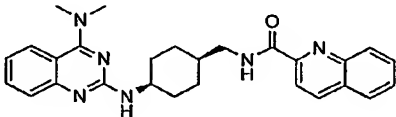
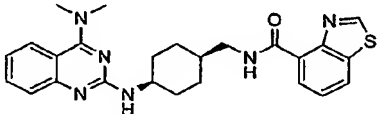
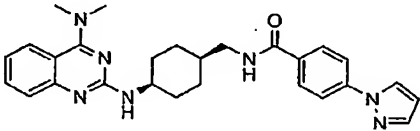
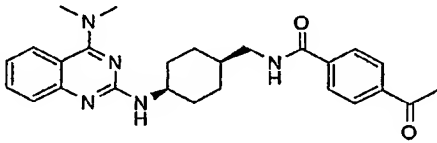
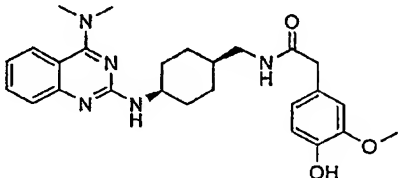
Example No.	Structure	ESI-MS	Retention Time (min)
3077	 <chem>COc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.61
3078	 <chem>COc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.86
3079	 <chem>CCCCCOc1ccc(cc1)C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.74
3080	 <chem>Fc1cc(F)c(F)cc1C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.68
3081	 <chem>C1CCCCC1C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.58
3082	 <chem>Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1C(=O)NCC2CCCCC2Nc3nc4ccccc4n(C)C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.4 (M + H)	4.19

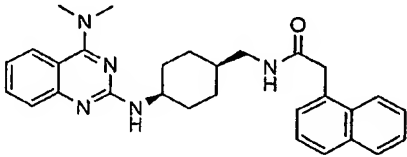
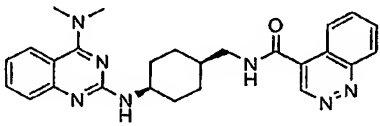
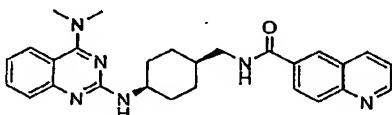
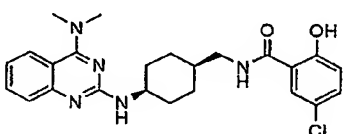
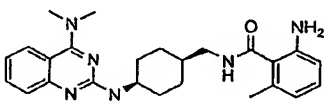
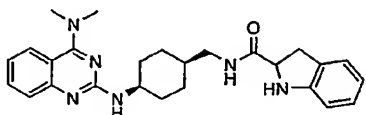
Example No.	Structure	ESI-MS	Retention Time (min)
3083	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3C(=O)Nc4ccc(F)cc4)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	3.50
3084	 <chem>COc1cc(OC)c(OC)c(C(=O)Nc2ccccc2N1N=C(NC3CCCCC3C(=O)Nc4cc(OC)c(OC)c(OC)c4)C5)c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	3.39
3085	 <chem>FC1=CC=C(C(=O)Nc2ccccc2N1N=C(NC3CCCCC3C(=O)Nc4cc(F)cc(F)c4)C5)=CC=C1F</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	3.55
3086	 <chem>Clc1ccccc1C(=O)Nc2ccccc2N1N=C(NC3CCCCC3C(=O)Nc4ccccc4C5)C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	438.2 (M + H)	3.48
3087	 <chem>c1ccc2cc(C(=O)Nc3ccccc3N1N=C(NC4CCCCC4C(=O)Nc5ccccc5C6)C2)ccc2ccccc26</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.75
3088	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3C(=O)Nc4ccc(C(F)(F)F)cc4)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.83

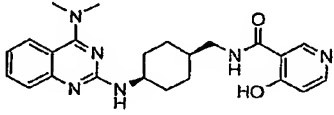
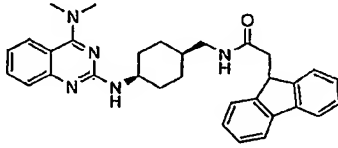
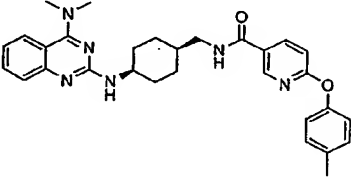
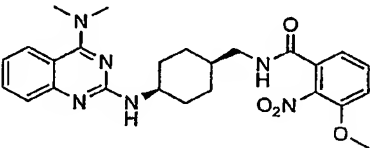
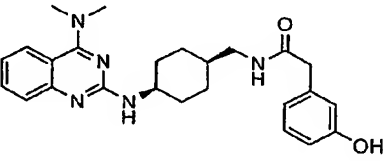
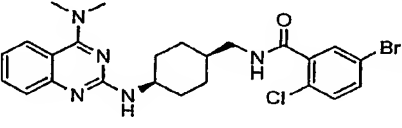
Example No.	Structure	ESI-MS	Retention Time (min)
3089	 <p>CF₃CO₂H</p>	422.2 (M + H)	3.51
3090	 <p>CF₃CO₂H</p>	472.4 (M + H)	3.87
3091	 <p>CF₃CO₂H</p>	500.4 (M + H)	3.03
3092	 <p>2CF₃CO₂H</p>	447.4 (M + H)	2.59
3093	 <p>CF₃CO₂H</p>	486.4 (M + H)	3.25
3094	 <p>CF₃CO₂H</p>	488.4 (M + H)	2.81

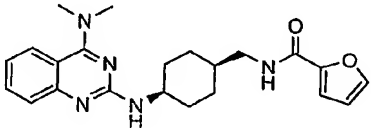
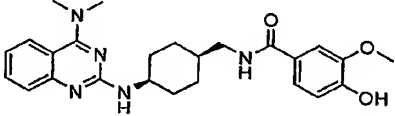
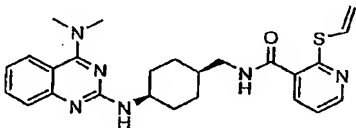
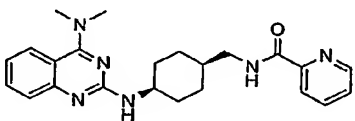
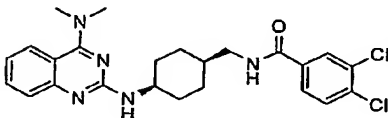
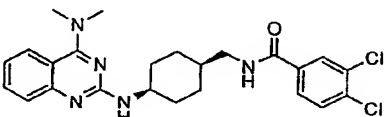
Example No.	Structure	ESI-MS	Retention Time (min)
3095	 <chem>CC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2N3C(=N)C(=NC4=CC=CC=C4N3C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	452.4 (M + H)	2.98
3096	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2N3C(=N)C(=NC4=CC=CC=C4N3C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.29
3097	 <chem>COC(=O)[C@H]1CCCC[C@H]1N2C(=N)C(=NC3=CC=CC=C3N2C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.77
3098	 <chem>O=C1C2=CC=CC=C2CCC1[C@H]3CCCC[C@H]3N4C(=N)C(=NC5=CC=CC=C5N4C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	3.06
3099	 <chem>O=C1C(=O)c2ccccc2O1[C@H]3CCCC[C@H]3N4C(=N)C(=NC5=CC=CC=C5N4C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	3.40
3100	 <chem>CC(=O)[C@H]1CCCC[C@H]1N2C(=N)C(=NC3=CC=CC=C3N2C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	2.69

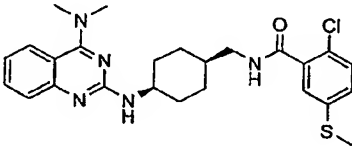
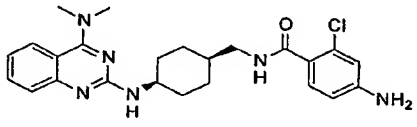
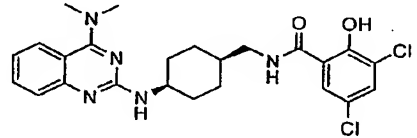
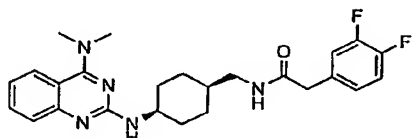
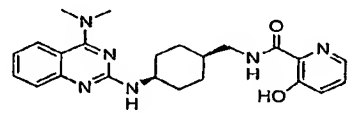
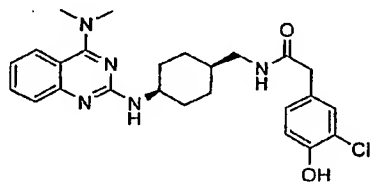
Example No.	Structure	ESI-MS	Retention Time (min)
3101	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CN(C)C(=N4)C5=CC=CC=C5)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.01
3102	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CC(=CC=C4C(=O)N)C(=O)N)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	2.79
3103	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CC(=CC=C4)C(=O)N)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.76
3104	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CC(=CC=C4C(=O)N)C(=O)N)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	3.03
3105	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CC(=CC=C4C(=O)N)C(=O)N)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.41
3106	 <chem>CC1=CN(C)C(=N1)N2C(=NC(=C2)C(=O)N[C@H]3CCCC[C@H]3C4=CC(=CC=C4C(=O)N)C(=O)N)C(=O)N</chem> $\text{CF}_3\text{CO}_2\text{H}$	483.2 (M + H)	2.84

Example No.	Structure	ESI-MS	Retention Time (min)
3107	 $2\text{CF}_3\text{CO}_2\text{H}$	455 (M + H)	2.45
3108	 $2\text{CF}_3\text{CO}_2\text{H}$	455.2 (M + H)	3.19
3109	 $\text{CF}_3\text{CO}_2\text{H}$	461.4 (M + H)	2.60
3110	 $2\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	2.74
3111	 $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	2.61
3112	 $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.35

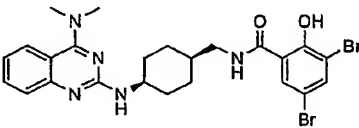
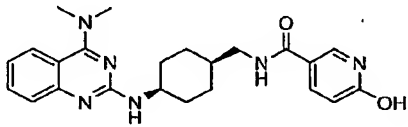
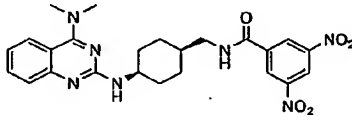
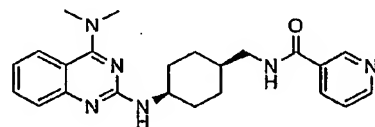
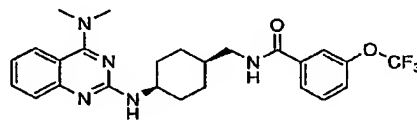
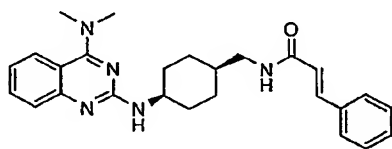
Example No.	Structure	ESI-MS	Retention Time (min)
3113	 <p>CF₃CO₂H</p>	468.4 (M + H)	3.04
3114	 <p>2CF₃CO₂H</p>	456.2 (M + H)	2.44
3115	 <p>2CF₃CO₂H</p>	455.2 (M + H)	2.11
3116	 <p>CF₃CO₂H</p>	454.2 (M + H)	3.21
3117	 <p>2CF₃CO₂H</p>	433.6 (M + H)	2.34
3118	 <p>2CF₃CO₂H</p>	444.6 (M+)	2.93

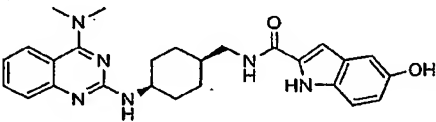
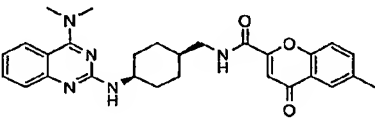
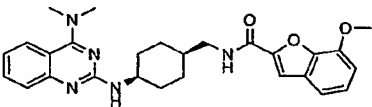
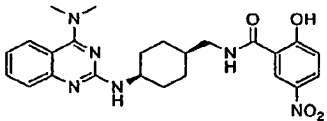
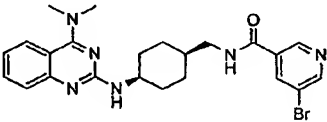
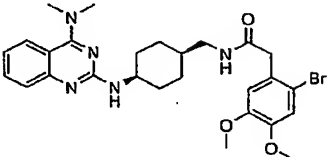
Example No.	Structure	ESI-MS	Retention Time (min)
3119	 2CF ₃ CO ₂ H	421.4 (M + H)	2.23
3120	 CF ₃ CO ₂ H	506.4 (M + H)	3.31
3121	 2CF ₃ CO ₂ H	511.6 (M + H)	3.21
3122	 CF ₃ CO ₂ H	479.4 (M + H)	3.60
3123	 CF ₃ CO ₂ H	434.4 (M + H)	2.37
3124	 CF ₃ CO ₂ H	516.4 (M + H)	3.02

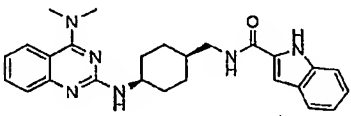
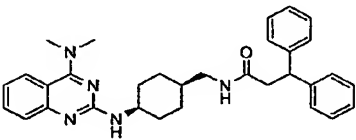
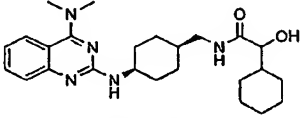
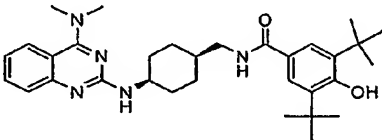
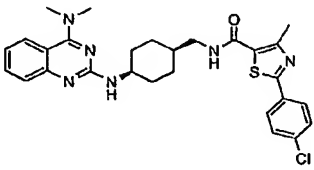
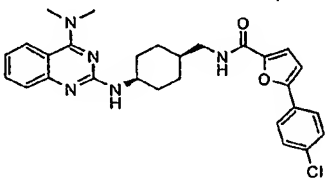
Example No.	Structure	ESI-MS	Retention Time (min)
3125	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC=CC=C4O</chem> $\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.45
3126	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC(=CC=C4)C(=O)OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.2 (M + H)	2.41
3127	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC=CC=C4S4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	477.0 (M + H)	2.88
3128	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC=CC=C4N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	2.61
3129	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC(=CC=C4)C(=O)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	472.6 (M + H)	3.17
3130	 <chem>CC1=CNC(=N2C=CC=CC=C2N1C)C[C@H]3CCCC[C@@H]3CNC(=O)C4=CC(=CC=C4)C(=O)Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.59

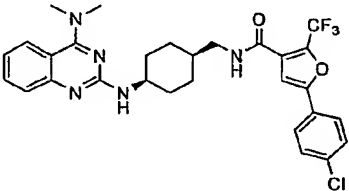
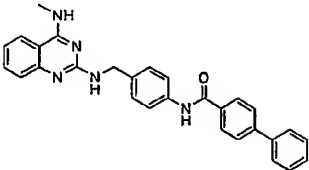
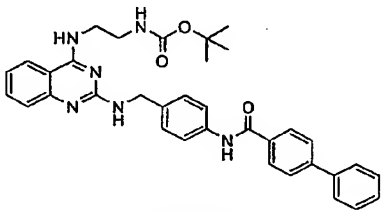
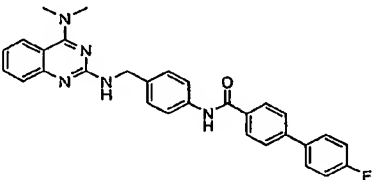
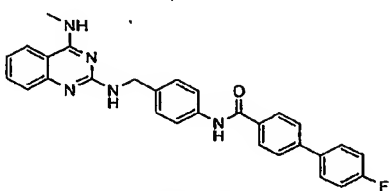
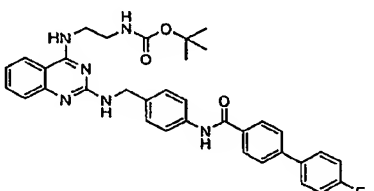
Example No.	Structure	ESI-MS	Retention Time (min)
3131	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5cc(Cl)cc(C)c5)N(C)N(C)N2C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	2.99
3132	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5cc(Cl)cc(N)c5)N(C)N(C)N2C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	453.0 (M + H)	2.45
3133	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5cc(Cl)c(O)c(Cl)c5)N(C)N(C)N2C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.59
3134	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5cc(F)c(F)cc5)N(C)N(C)N2C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.81
3135	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5ccncc5O)N(C)N(C)N2C1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	421.4 (M + H)	2.89
3136	 <chem>CC1=CC=C2N3C(NC4CCCCC4CC(=O)Nc5cc(Cl)c(O)cc5)N(C)N(C)N2C1</chem> $\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.53

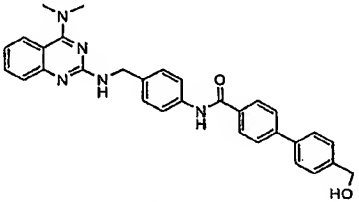
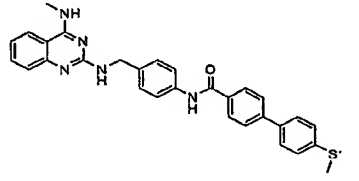
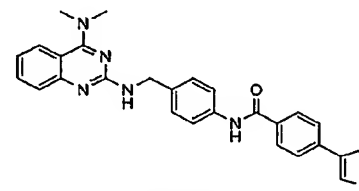
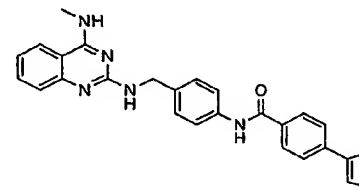
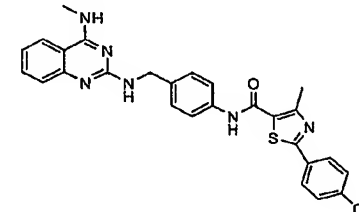
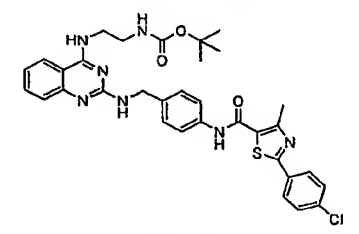
Example No.	Structure	ESI-MS	Retention Time (min)
3137	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3cc(N)c(Cl)cc3OC</chem> 2CF ₃ CO ₂ H	483.2 (M + H)	2.83
3138	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3ccc(s3)-c4ccccc4</chem> CF ₃ CO ₂ H	487.4 (M+2H ⁺)	3.40
3139	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3c[nH]sc3S</chem> CF ₃ CO ₂ H	445.6 (M + H)	2.36
3140	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3cc(N)c(Cl)cc3</chem> 2CF ₃ CO ₂ H	453.2 (M + H)	2.46
3141	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3cc(OC)cc(OC)c3OC</chem> CF ₃ CO ₂ H	478.4 (M + H)	2.77
3142	 <chem>CN(C)c1nc2c(ncn2C1)NC(=O)Cc3cc(O)c(I)cc3</chem> CF ₃ CO ₂ H	672.2 (M + H)	3.92

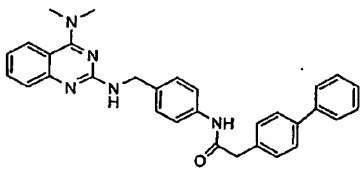
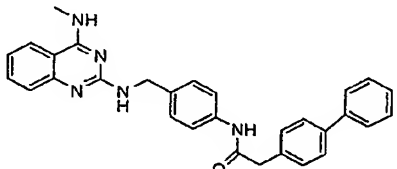
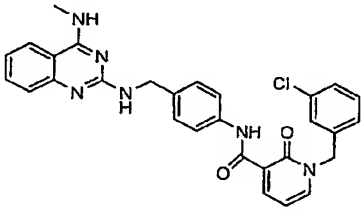
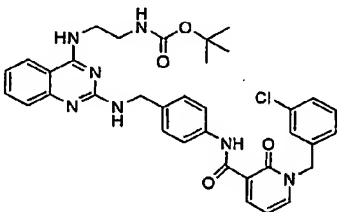
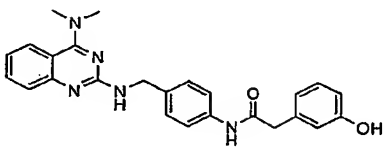
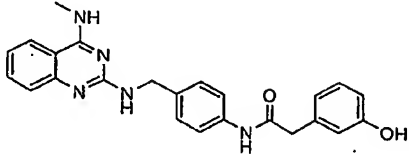
Example No.	Structure	ESI-MS	Retention Time (min)
3143	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC(=CC=C7)C(=O)NCC8=CC=C(C=C8)BrC9=CC=C(C=C9)Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	576.2 (M + H)	3.71
3144	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC=CC=C7C(=O)NCC8=CC=CC=C8C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	421.2 (M + H)	2.01
3145	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC(=CC=C7)C(=O)NCC8=CC=CC=C8C(=O)[N+](=O)[O-]</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.77
3146	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC=CC=C7C(=O)NCC8=CC=CC=C8</chem> $2\text{CF}_3\text{CO}_2\text{H}$	405.6 (M + H)	1.99
3147	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC(=CC=C7)C(=O)NCC8=CC=CC=C8OC(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	488.4 (M + H)	3.13
3148	 <chem>CC1=NC2=CC=CC=C2N1C3=CC=CC=C3N3C4=CC=CC=C4C5=CC=CC=C5N5C6=CC=CC=C6C7=CC=CC=C7C(=O)NCC8=CC=CC=C8C(=O)C=C9=CC=CC=C9</chem> $\text{CF}_3\text{CO}_2\text{H}$	430.4 (M + H)	2.91

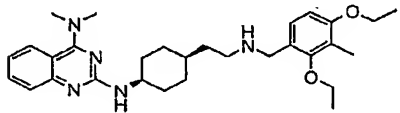
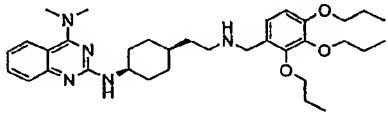
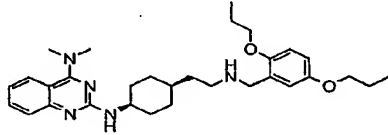
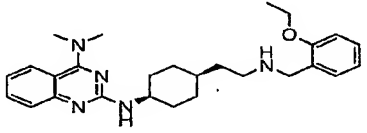
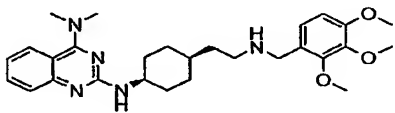
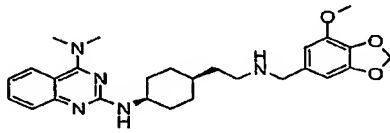
Example No.	Structure	ESI-MS	Retention Time (min)
3149	 $2\text{CF}_3\text{CO}_2\text{H}$	459.4 (M + H)	2.47
3150	 $\text{CF}_3\text{CO}_2\text{H}$	486.6 (M + H)	2.93
3151	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.03
3152	 $\text{CF}_3\text{CO}_2\text{H}$	465.2 (M + H)	3.13
3153	 $2\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	2.67
3154	 $\text{CF}_3\text{CO}_2\text{H}$	556.4 (M + H)	2.84

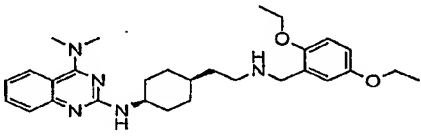
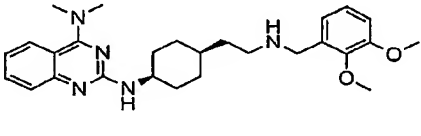
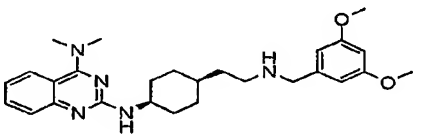
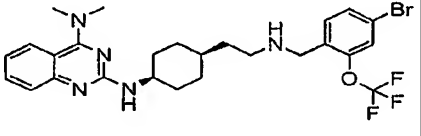
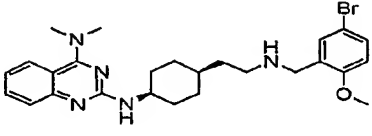
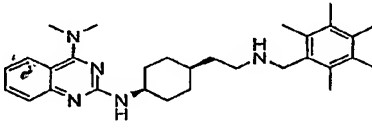
Example No.	Structure	ESI-MS	Retention Time (min)
3155	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)c4c[nH]c5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	443.4 (M + H)	2.94
3156	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)C(c1ccccc1)C(=O)c2ccccc2</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.20
3157	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)C4CCCCC4C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.0 (M + H)	2.72
3158	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)C4=C(C(C)(C)O)C(C)(C)C=C4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	532.4 (M + H)	3.58
3159	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)c4nc5ccc(Cl)cc5s4</chem> $\text{CF}_3\text{CO}_2\text{H}$	535.4 (M + H)	3.51
3160	 <chem>CC1=NC2=CC=CC=C2N(C)N1CCN3CCCCC3CCNC(=O)c4oc5ccc(Cl)cc5c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	3.49

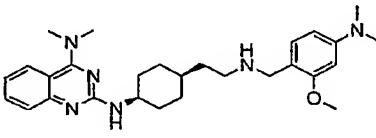
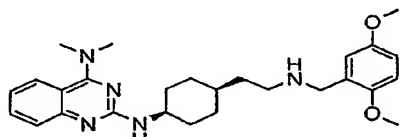
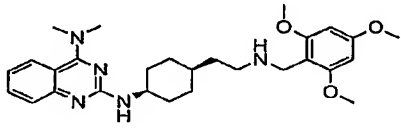
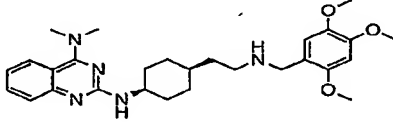
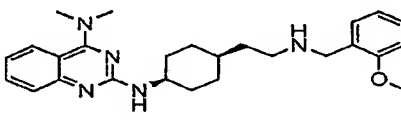
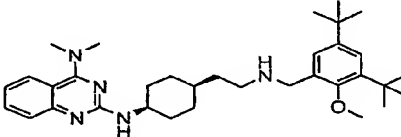
Example No.	Structure	ESI-MS	Retention Time (min)
3161	 <chem>CC1=NC2=CC=CC=C2N(C)N1CC3CCCCC3CC(=O)C4=C(C(F)(F)F)OC(C4)C5=CC=C(C=C5)Cl</chem> <chem>CF3CO2H</chem>	572.4 (M + H)	3.71
3162	 <chem>CN1=NC2=CC=CC=C2N=CN1CC3=CC=CC=C3CC(=O)Nc4ccc(cc4)C5=CC=CC=C5</chem> <chem>CF3CO2H</chem>	460.2 (M + H)	3.80
3163	 <chem>CC(C)(C)OC(=O)NCCN1=NC2=CC=CC=C2N=CN1CC3=CC=CC=C3CC(=O)Nc4ccc(cc4)C5=CC=CC=C5</chem> <chem>CF3CO2H</chem>	589.2 (M + H)	4.00
3164	 <chem>CN1=NC2=CC=CC=C2N=CN1CC3=CC=CC=C3CC(=O)Nc4ccc(cc4)C5=CC=C(C=C5)F</chem> <chem>CF3CO2H</chem>	492.2 (M + H)	3.90
3165	 <chem>CN1=NC2=CC=CC=C2N=CN1CC3=CC=CC=C3CC(=O)Nc4ccc(cc4)C5=CC=C(C=C5)F</chem> <chem>CF3CO2H</chem>	478.2 (M + H)	3.80
3166	 <chem>CC(C)(C)OC(=O)NCCN1=NC2=CC=CC=C2N=CN1CC3=CC=CC=C3CC(=O)Nc4ccc(cc4)C5=CC=C(C=C5)F</chem> <chem>CF3CO2H</chem>	607.6 (M + H)	4.00

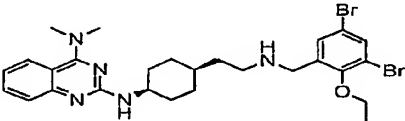
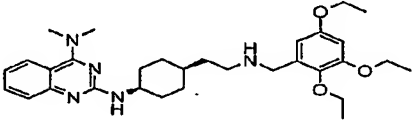
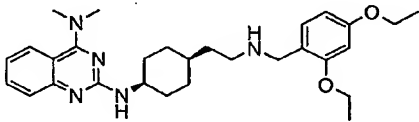
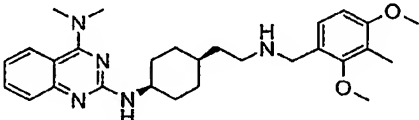
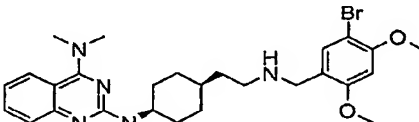
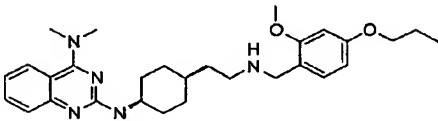
Example No.	Structure	ESI-MS	Retention Time (min)
3167	 <chem>CCN(C)c1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc(O)cc4)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.40
3168	 <chem>C[Si](C)(C)c1ccc(NC(=O)c2ccc(CNc3nc4ccccc4n3)cc2)cc1</chem> $\text{CF}_3\text{CO}_2\text{H}$	506.2 (M + H)	3.90
3169	 <chem>CCN(C)c1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc5ccsc54)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	3.80
3170	 <chem>CNc1nc2ccccc2n1CNc3ccc(NC(=O)c4ccc5ccsc54)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.70
3171	 <chem>CNc1nc2ccccc2n1CNc3ccc(NC(=O)c4nn(s4)c5ccc(Cl)cc5)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	515.2 (M + H)	3.90
3172	 <chem>CC(C)(C)OC(=O)Nc1nc2ccccc2n1CNc3ccc(NC(=O)c4nn(s4)c5ccc(Cl)cc5)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	4.10

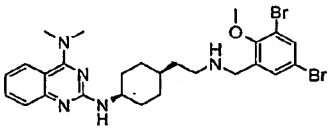
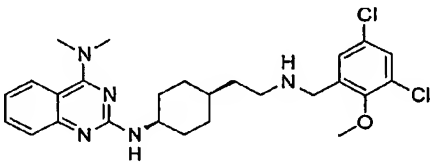
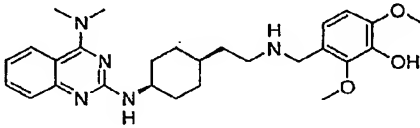
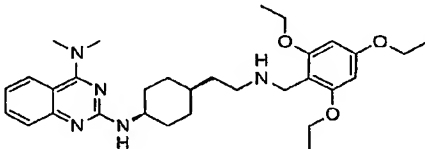
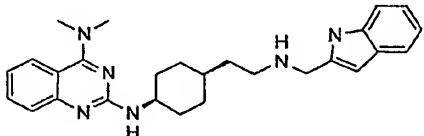
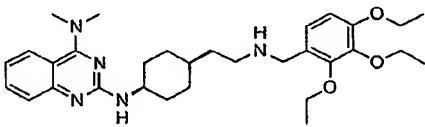
Example No.	Structure	ESI-MS	Retention Time (min)
3173	 CF ₃ CO ₂ H	488.2 (M + H)	3.90
3174	 CF ₃ CO ₂ H	474.4 (M + H)	3.80
3175	 CF ₃ CO ₂ H	525.4 (M + H)	3.70
3176	 CF ₃ CO ₂ H	654.2 (M + H)	3.90
3177	 CF ₃ CO ₂ H	428.2 (M + H)	3.10
3178	 CF ₃ CO ₂ H	414.4 (M + H)	2.90

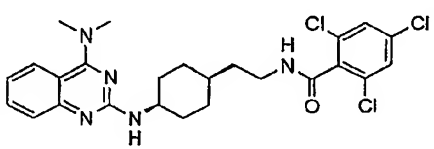
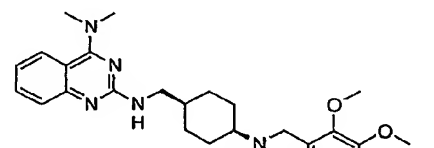
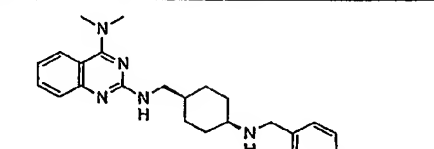
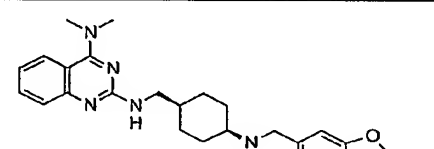
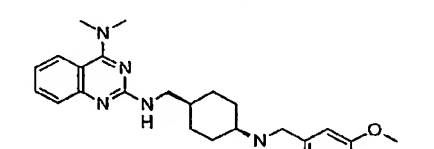
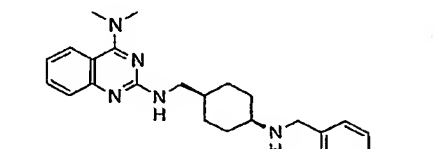
Example No.	Structure	ESI-MS	Retention Time (min)
3179	 $2\text{CF}_3\text{CO}_2\text{H}$	506.4 (M + H)	3.04
3180	 $2\text{CF}_3\text{CO}_2\text{H}$	578.8 (M + H)	3.50
3181	 $2\text{CF}_3\text{CO}_2\text{H}$	520.6 (M + H)	3.19
3182	 $2\text{CF}_3\text{CO}_2\text{H}$	448.4 (M + H)	2.80
3183	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.66
3184	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.66

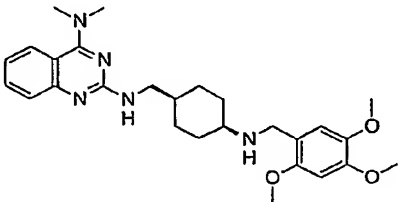
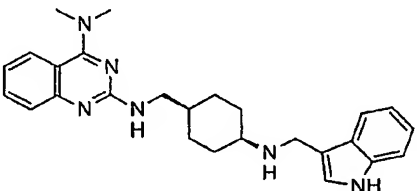
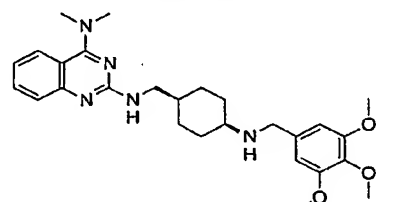
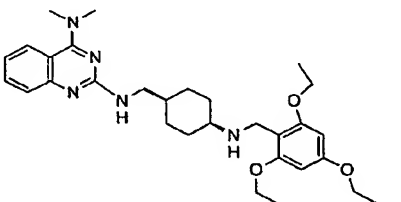
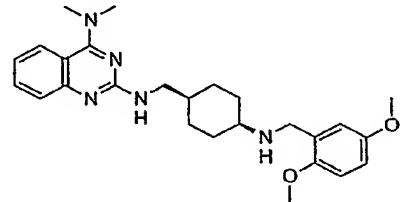
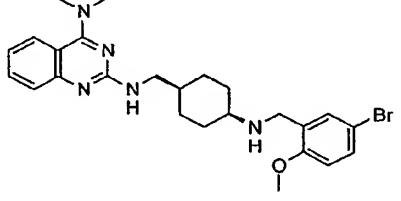
Example No.	Structure	ESI-MS	Retention Time (min)
3185	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5ccc(OC)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.94
3186	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5cc(OC)c(OC)cc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.65
3187	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5cc(OC)cc(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.68
3188	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5ccc(Br)cc5OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	566.4 (M + H)	3.03
3189	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5cc(Br)cc(OC)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	512.6 (M + H)	2.85
3190	 <chem>CC1=CC=C(C=C1)N2C(=NC3=CC=CC=C3N(C)N2)N[C@H]4CCCC[C@H]4CNCCc5c(C)c(C)c(C)c5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	3.09

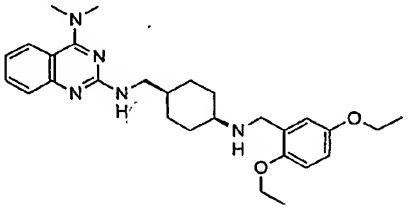
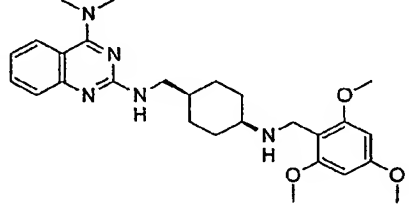
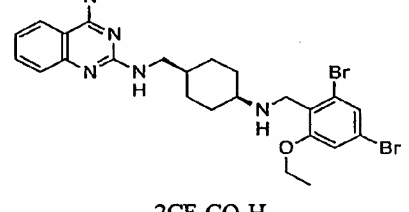
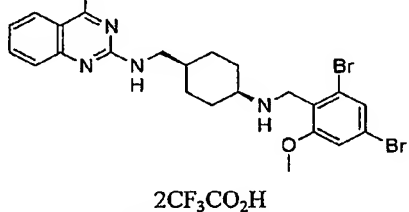
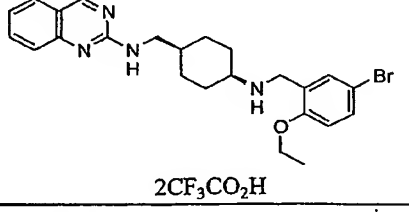
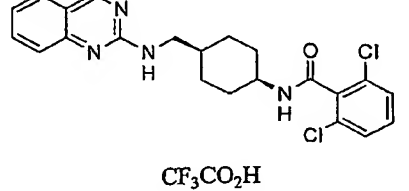
Example No.	Structure	ESI-MS	Retention Time (min)
3191	 $3\text{CF}_3\text{CO}_2\text{H}$	477.4 (M + H)	2.51
3192	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	2.67
3193	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.78
3194	 $2\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.60
3195	 $2\text{CF}_3\text{CO}_2\text{H}$	434.6 (M + H)	2.67
3196	 $2\text{CF}_3\text{CO}_2\text{H}$	546.4 (M + H)	4.30

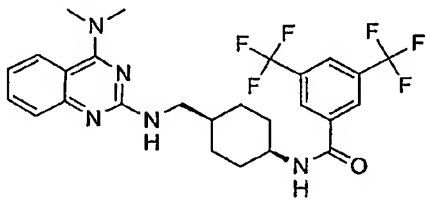
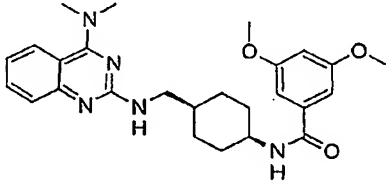
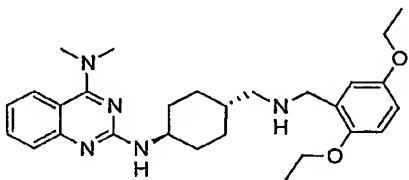
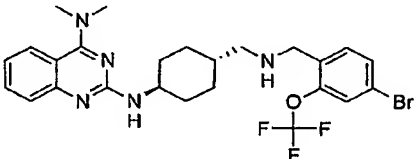
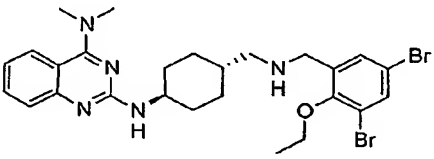
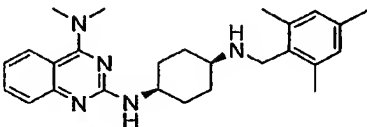
Example No.	Structure	ESI-MS	Retention Time (min)
3197	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(Br)=C(Br)C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	606.6 (M + H)	3.95
3198	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(OC)=C(OC)C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	536.6 (M + H)	3.83
3199	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(OC)=CC4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.4 (M + H)	2.97
3200	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(OC)=CC4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	2.79
3201	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(Br)=C(OC)C4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	542.0 (M + H)	2.85
3202	 <chem>CC1=CN2C(=N1)N(C)C=N2C(=O)N[C@H]3CCCC[C@H]3CCNCC4=CC(=C(C=C4)OC)C(OC)=CC4OCC</chem> $2\text{CF}_3\text{CO}_2\text{H}$	492.6 (M + H)	2.81

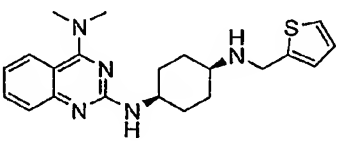
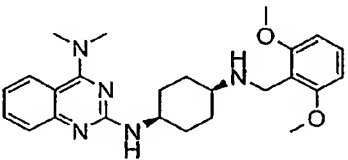
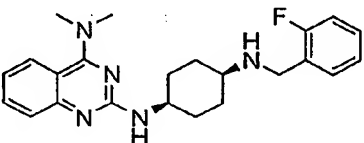
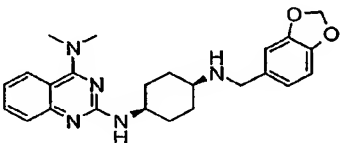
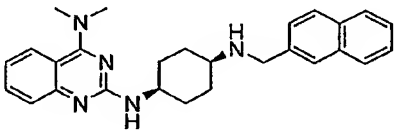
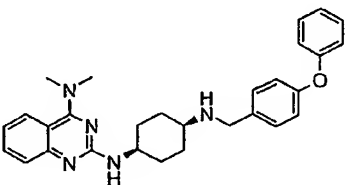
Example No.	Structure	ESI-MS	Retention Time (min)
3203	 $2\text{CF}_3\text{CO}_2\text{H}$	590.4 (M + H)	3.02
3204	 $2\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	2.91
3205	 $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.51
3206	 $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.21
3207	 $3\text{CF}_3\text{CO}_2\text{H}$	443.6 (M + H)	2.66
3208	 $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.08

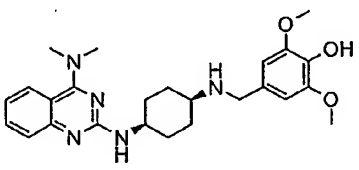
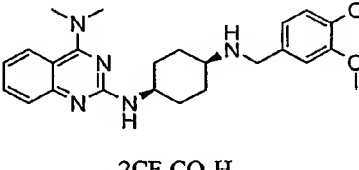
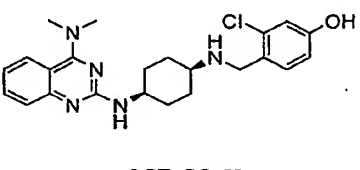
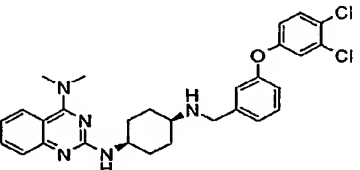
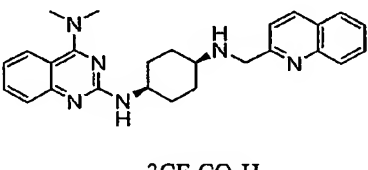
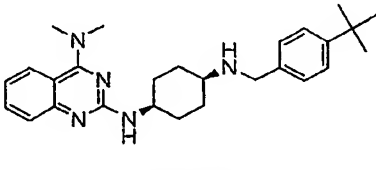
Example No.	Structure	ESI-MS	Retention Time (min)
3209	 $2\text{CF}_3\text{CO}_2\text{H}$	520.0 (M + H)	3.51
3210	 $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.58
3211	 $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.11
3212	 $2\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.22
3213	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.70
3214	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.58

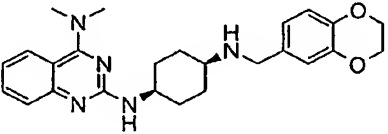
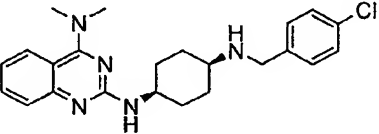
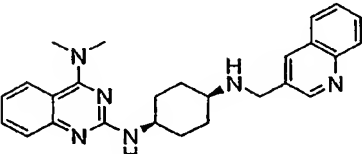
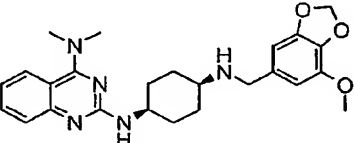
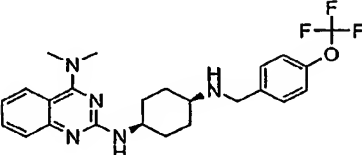
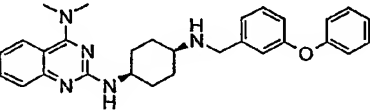
Example No.	Structure	ESI-MS	Retention Time (min)
3215	 $2\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	2.73
3216	 $3\text{CF}_3\text{CO}_2\text{H}$	429.4 (M + H)	3.29
3217	 $2\text{CF}_3\text{CO}_2\text{H}$	480.2 (M + H)	2.78
3218	 $2\text{CF}_3\text{CO}_2\text{H}$	522.4 (M + H)	3.77
3219	 $2\text{CF}_3\text{CO}_2\text{H}$	450.2 (M + H)	2.57
3220	 $2\text{CF}_3\text{CO}_2\text{H}$	498.0 (M + H)	2.97

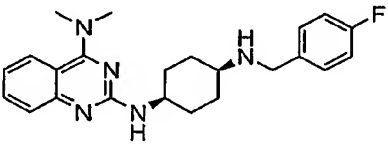
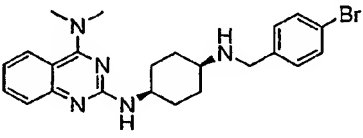
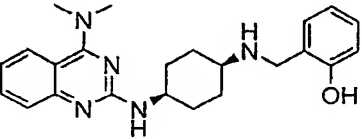
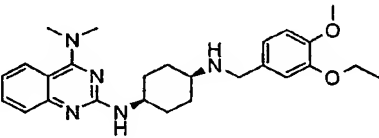
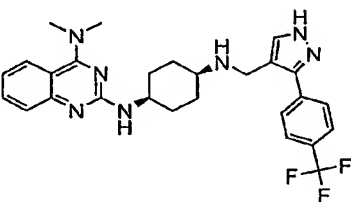
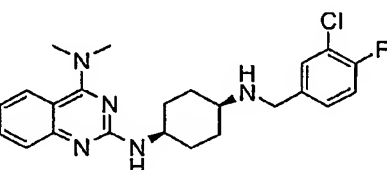
Example No.	Structure	ESI-MS	Retention Time (min)
3221	 $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.17
3222	 $2\text{CF}_3\text{CO}_2\text{H}$	480.0 (M + H)	3.08
3223	 $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	4.20
3224	 $2\text{CF}_3\text{CO}_2\text{H}$	576.4 (M + H)	3.95
3225	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.86
3226	 $\text{CF}_3\text{CO}_2\text{H}$	472.4 (M + H)	3.07

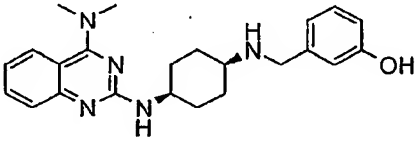
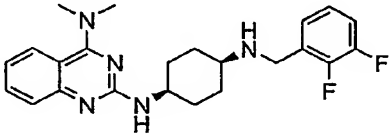
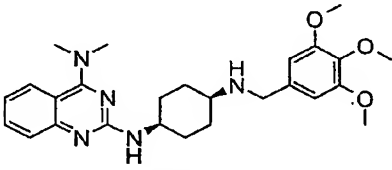
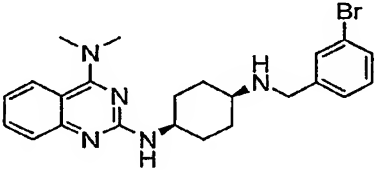
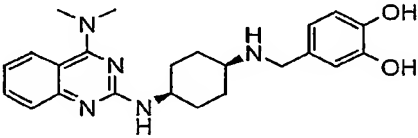
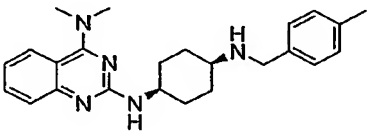
Example No.	Structure	ESI-MS	Retention Time (min)
3227	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3NC(=O)c4ccc(C(F)(F)F)cc4)N1C</chem> $\text{CF}_3\text{CO}_2\text{H}$	540.6 (M + H)	3.75
3228	 <chem>COc1ccc(NC(=O)C2CCCCC2NC3=NC4=CC=CC=C4N(C)C3=N)cc1OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.4 (M + H)	3.07
3229	 <chem>CCOC1=CC=C(C=C1C2=CC=CC=C2N(C)C2)NCC3CCCCC3NC4=NC5=CC=CC=C5N(C)C4=N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.4 (M + H)	3.40
3230	 <chem>BrC1=CC=C(C=C1C2=CC=CC=C2N(C)C2)NCC3CCCCC3NC4=NC5=CC=CC=C5N(C)C4=N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.6 (M + H)	3.50
3231	 <chem>CCOC1=CC=C(C=C1C2=CC=CC=C2N(C)C2)NCC3CCCCC3NC4=NC5=CC=CC=C5N(C)C4=N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	590.2 (M + H)	3.60
3232	 <chem>CC1=CC=C(C=C1C2=CC=CC=C2N(C)C2)NCC3CCCCC3NC4=NC5=CC=CC=C5N(C)C4=N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.25

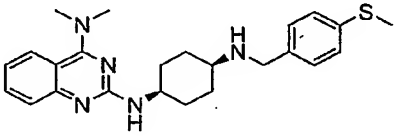
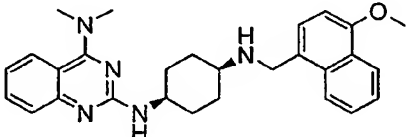
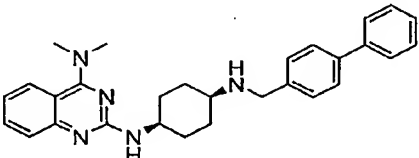
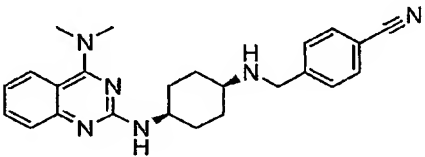
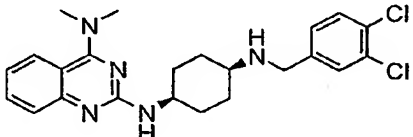
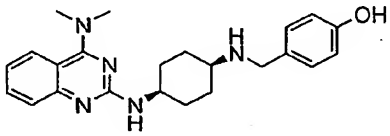
Example No.	Structure	ESI-MS	Retention Time (min)
3233	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4ccsc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	382.2 (M + H)	2.67
3234	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4cc(OC)c(OC)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	3.05
3235	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4ccccc4F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.75
3236	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4ccc5c(c4)OCO5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.82
3237	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4ccc5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.4 (M + H)	3.17
3238	 <chem>CN1C=NC2=C(N1)C=CC=C2N[C@H]3CCCC[C@H]3NCc4ccc(Oc5ccccc5)cc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.44

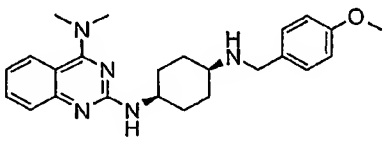
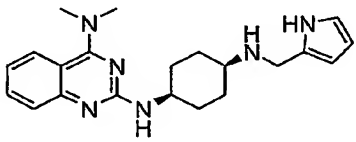
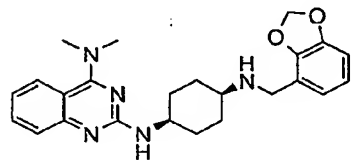
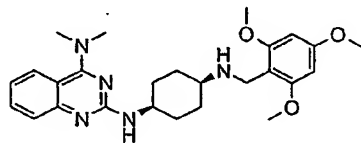
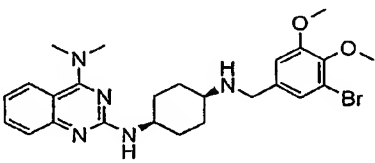
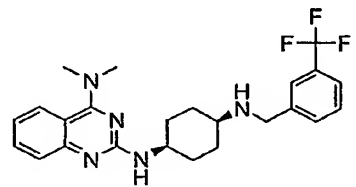
Example No.	Structure	ESI-MS	Retention Time (min)
3239	 $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	2.69
3240	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.80
3241	 $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	2.79
3242	 $2\text{CF}_3\text{CO}_2\text{H}$	536.4 (M + H)	3.75
3243	 $3\text{CF}_3\text{CO}_2\text{H}$	427.2 (M + H)	2.95
3244	 $2\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.41

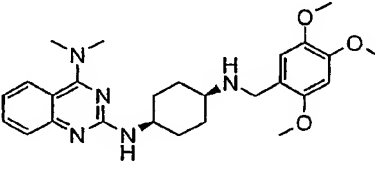
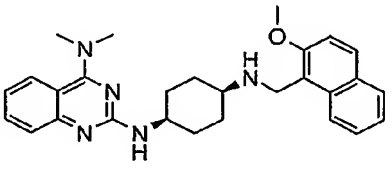
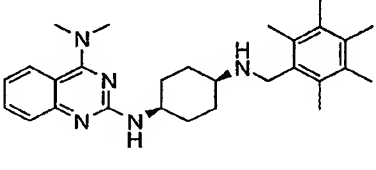
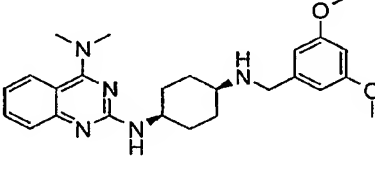
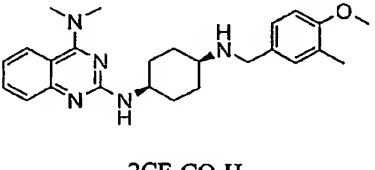

Example No.	Structure	ESI-MS	Retention Time (min)
3245	 $2\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	2.84
3246	 $2\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.02
3247	 $3\text{CF}_3\text{CO}_2\text{H}$	427.4 (M + H)	2.61
3248	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.91
3249	 $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.19
3250	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	2.79

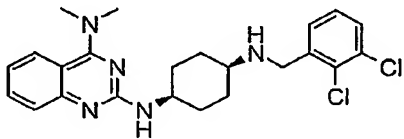
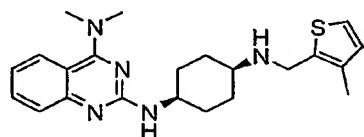
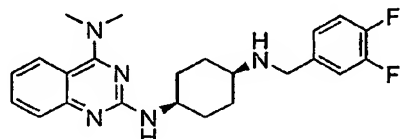
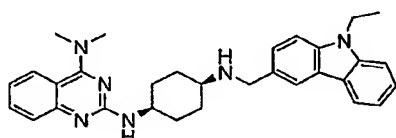
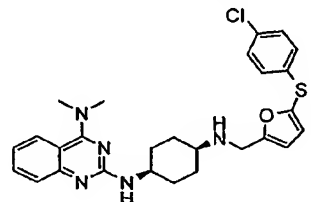
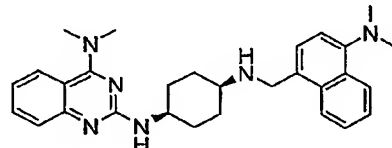
Example No.	Structure	ESI-MS	Retention Time (min)
3251	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4ccc(F)cc4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.83
3252	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4ccc(Br)cc4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.08
3253	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4cc(O)ccc4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.73
3254	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4cc(OC)c(OC)cc4)cc3ccccc13</chem> $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.92
3255	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4cc5nn[nH]5C(c4)C6=CC=C(C(=C6)C(F)(F)F)C7=CC=CC=C7</chem> $3\text{CF}_3\text{CO}_2\text{H}$	510.4 (M + H)	3.17
3256	 <chem>CN(C)c1nc2c(ncn2C1N[C@H]3CCCC[C@H]3NCc4cc(F)ccc4Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	428.2 (M + H)	3.08

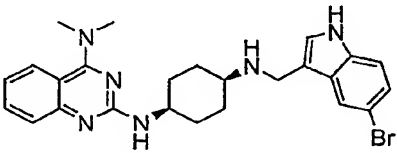
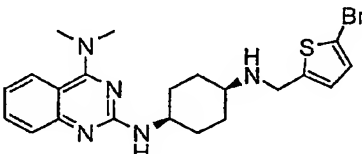
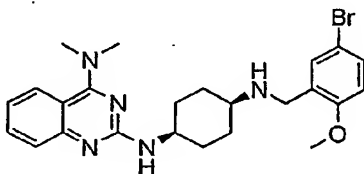
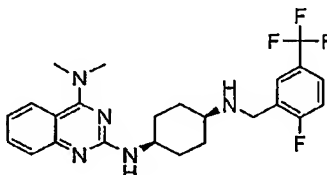
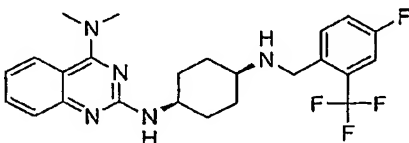
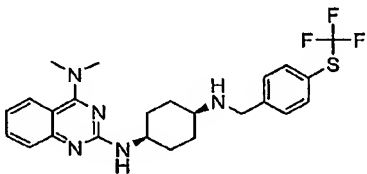
Example No.	Structure	ESI-MS	Retention Time (min)
3257	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(O)cc4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	392.4 (M + H)	2.63
3258	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(F)c(F)cc4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	412.2 (M + H)	2.83
3259	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(OC)c(OC)c(OC)c4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	2.89
3260	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(Br)cc4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	3.05
3261	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4cc(O)c(O)cc4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	2.53
3262	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCc4ccc(C)cc4)c5ccccc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.92

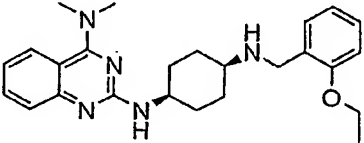
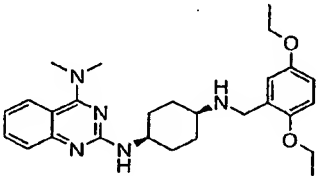
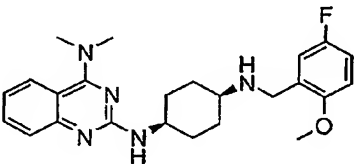
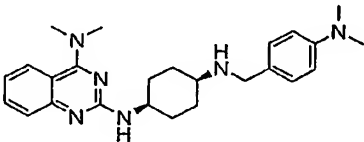
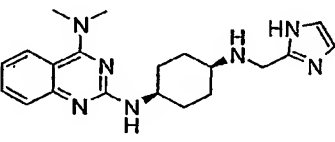
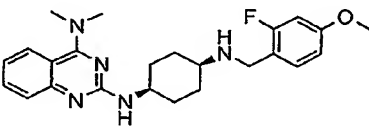
Example No.	Structure	ESI-MS	Retention Time (min)
3263	 2CF ₃ CO ₂ H	422.2 (M + H)	3.05
3264	 2CF ₃ CO ₂ H	456.4 (M + H)	3.25
3265	 2CF ₃ CO ₂ H	452.2 (M + H)	3.37
3266	 2CF ₃ CO ₂ H	401.2 (M + H)	2.76
3267	 2CF ₃ CO ₂ H	444.4 (M + H)	3.17
3268	 2CF ₃ CO ₂ H	392.4 (M + H)	2.61

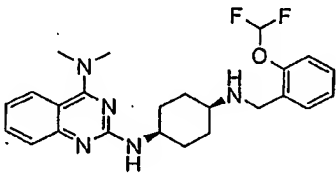
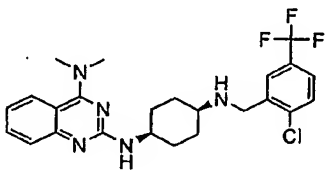
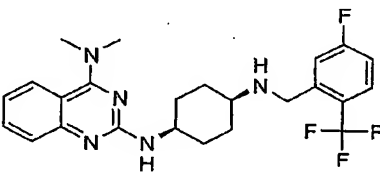
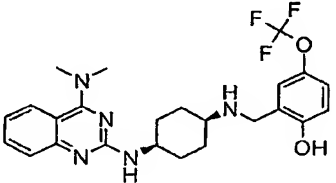
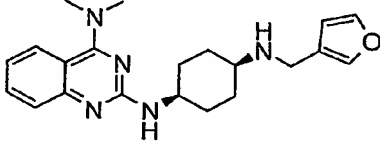
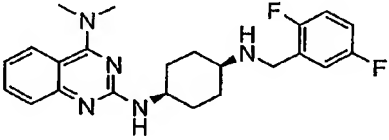
Example No.	Structure	ESI-MS	Retention Time (min)
3269	 $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.86
3270	 $3\text{CF}_3\text{CO}_2\text{H}$	365.4 (M + H)	2.61
3271	 $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.83
3272	 $2\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.10
3273	 $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.13
3274	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.17

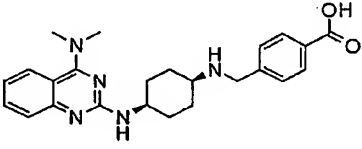
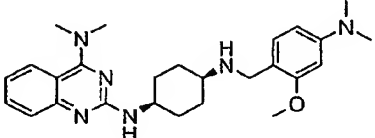
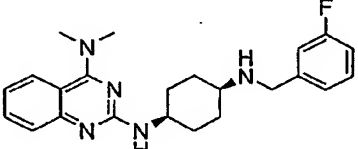
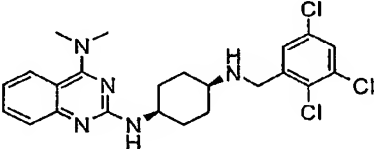
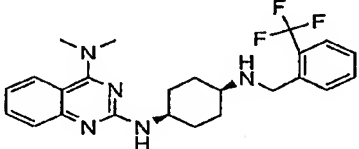
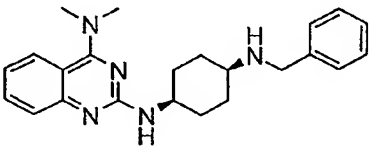
Example No.	Structure	ESI-MS	Retention Time (min)
3275	 2CF ₃ CO ₂ H	466.4 (M + H)	2.86
3276	 2CF ₃ CO ₂ H	456.2 (M + H)	3.22
3277	 2CF ₃ CO ₂ H	446.6 (M + H)	3.45
3278	 2CF ₃ CO ₂ H	436.4 (M + H)	2.95
3279	 2CF ₃ CO ₂ H	420.2 (M + H)	3.03
3280	 2CF ₃ CO ₂ H	382.4 (M + H)	2.72

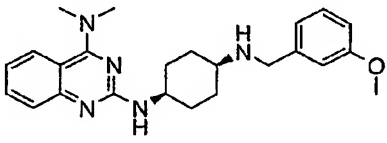
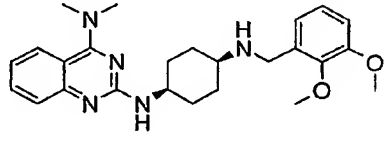
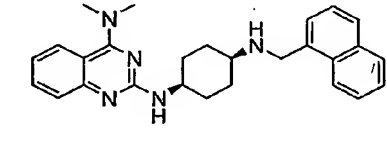
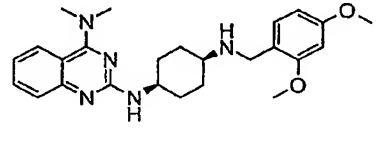
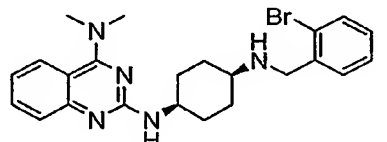
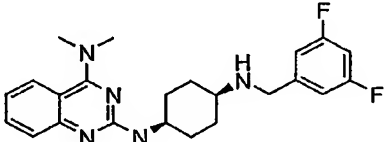
Example No.	Structure	ESI-MS	Retention Time (min)
3281	 $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.07
3282	 $2\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	2.79
3283	 $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.95
3284	 $32\text{CF}_3\text{CO}_2\text{H}$	493.4 (M + H)	3.57
3285	 $2\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.52
3286	 $2\text{CF}_3\text{CO}_2\text{H}$	469.6 (M + H)	2.76

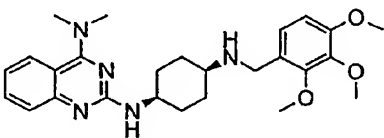
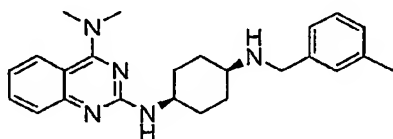
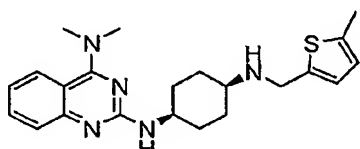
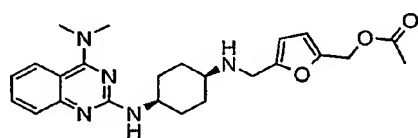
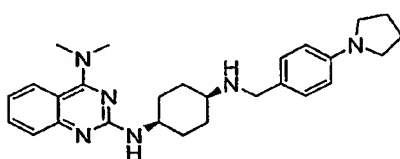
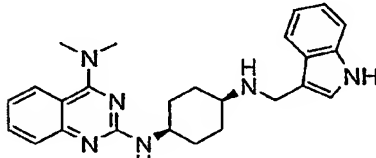
Example No.	Structure	ESI-MS	Retention Time (min)
3287	 $3\text{CF}_3\text{CO}_2\text{H}$	493.2 (M + H)	3.17
3288	 $2\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	2.95
3289	 $2\text{CF}_3\text{CO}_2\text{H}$	484.2 (M + H)	3.14
3290	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.11
3291	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.11
3292	 $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.39

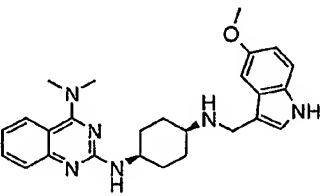
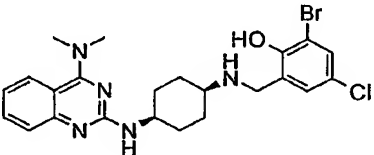
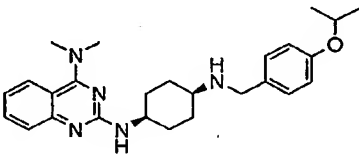
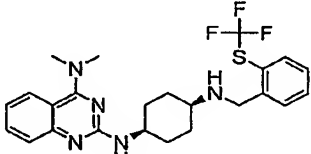
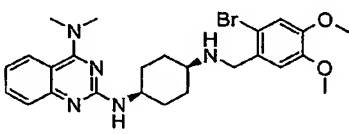
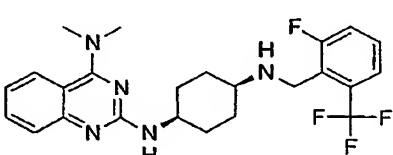
Example No.	Structure	ESI-MS	Retention Time (min)
3293	 <chem>CCOC1=CC=C(C=C1)N[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	3.05
3294	 <chem>CCOC1=CC(OC)=C(C=C1)N[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	3.21
3295	 <chem>COc1ccc(F)cc1N[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.94
3296	 <chem>CN(C)c1ccc(CN[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N)cc1</chem> $3\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	2.51
3297	 <chem>C1=CN=C(C=N1)CN[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N</chem> $3\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.26
3298	 <chem>COc1ccc(F)cc1N[C@H]2CC[C@@H](C2)N[C@H]3C(=NC4=CC=CC=C4N(C)C5=CC=CC=C35)N</chem> $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.93

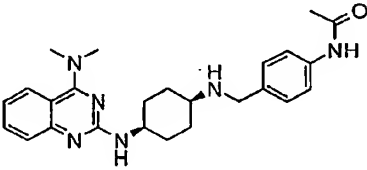
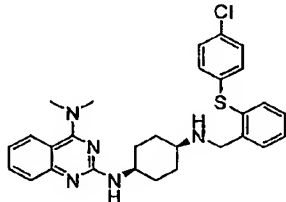
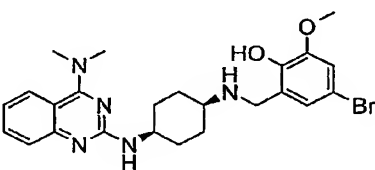
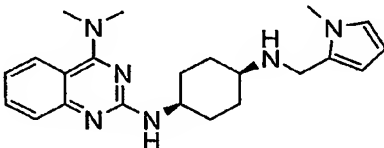
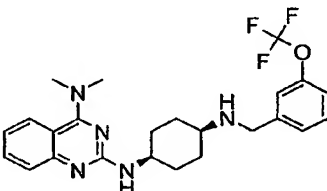
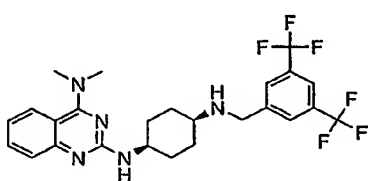
Example No.	Structure	ESI-MS	Retention Time (min)
3299	 $2\text{CF}_3\text{CO}_2\text{H}$	442.4 (M + H)	2.97
3300	 $2\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.19
3301	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.05
3302	 $2\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.20
3303	 $2\text{CF}_3\text{CO}_2\text{H}$	366.4 (M + H)	2.64
3304	 $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.85

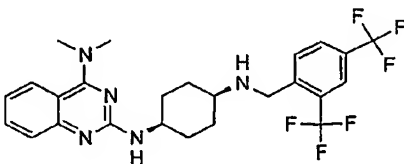
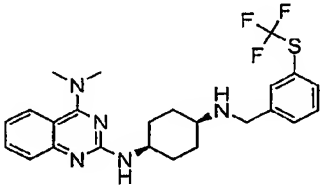
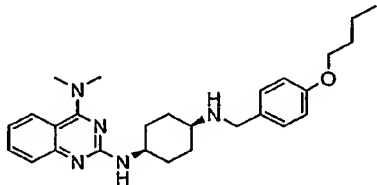
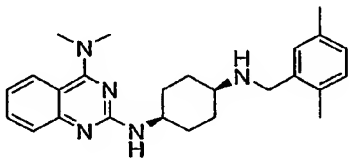
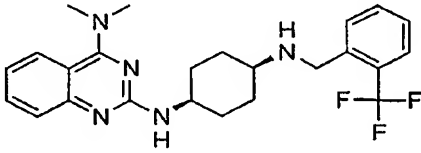
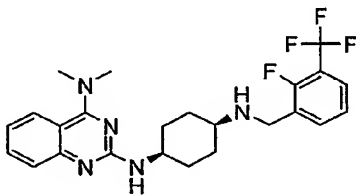
Example No.	Structure	ESI-MS	Retention Time (min)
3305	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.67
3306	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $3\text{CF}_3\text{CO}_2\text{H}$	449.4 (M + H)	2.74
3307	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	394.4 (M + H)	2.86
3308	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	478.2 (M + H)	3.38
3309	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.09
3310	 <chem>CN(C)c1nc2c(ncn2C1)C(=O)O</chem> $2\text{CF}_3\text{CO}_2\text{H}$	376.4 (M + H)	2.82

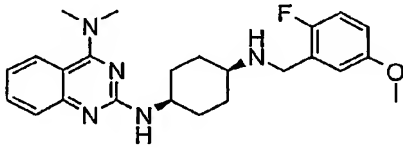
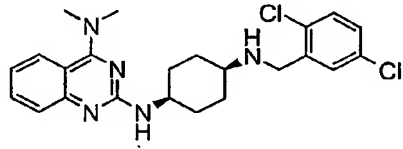
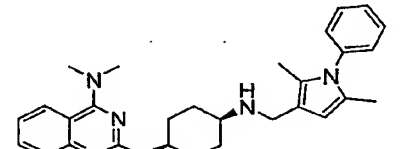
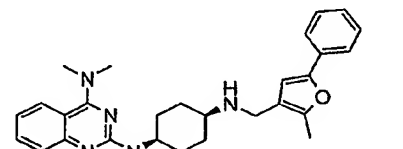
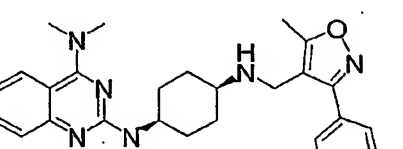
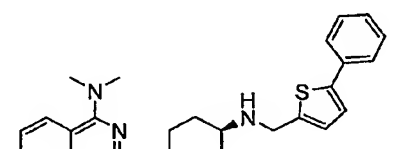
Example No.	Structure	ESI-MS	Retention Time (min)
3311	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC=C(C=C5)OC)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.87
3312	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC(OC)=CC(OC)=C5)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.91
3313	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC6=CC=CC=C6C=C5)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.13
3314	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC(OC)=CC(OC)=C5)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.99
3315	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC=C(C=C5)Br)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	454.0 (M + H)	2.97
3316	 <chem>CN(C)c1nc2c(nc3ccccc13)nc(NC4CCCCC4NC5=CC(F)=CC(F)=C5)nc2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	412.4 (M + H)	2.92

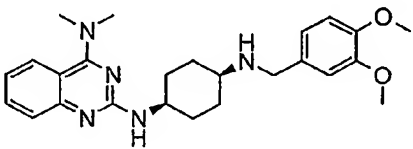
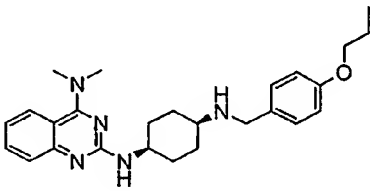
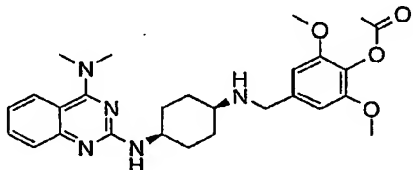
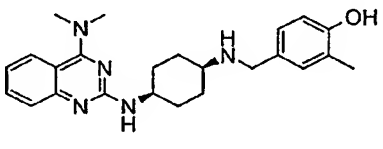
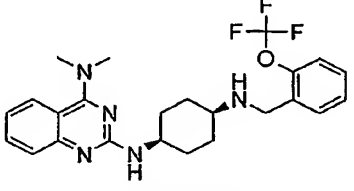
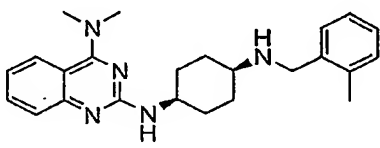
Example No.	Structure	ESI-MS	Retention Time (min)
3317	 2CF ₃ CO ₂ H	466.4 (M + H)	2.95
3318	 2CF ₃ CO ₂ H	390.4 (M + H)	2.95
3319	 2CF ₃ CO ₂ H	396.2 (M + H)	2.89
3320	 2CF ₃ CO ₂ H	438.2 (M + H)	2.76
3321	 3CF ₃ CO ₂ H	445.4 (M + H)	3.16
3322	 3CF ₃ CO ₂ H	415.4 (M + H)	2.96

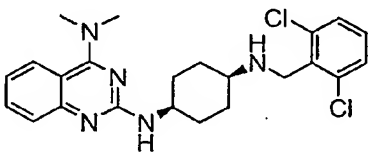
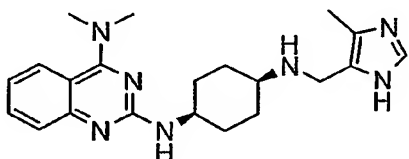
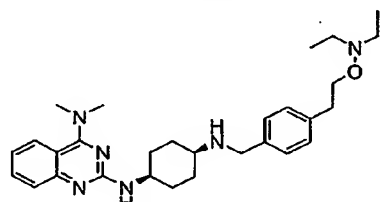
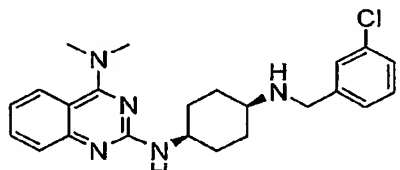
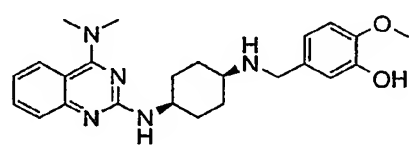
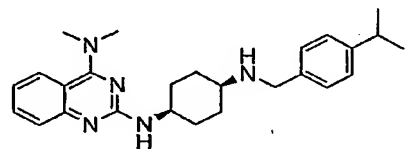
Example No.	Structure	ESI-MS	Retention Time (min)
3323	 <chem>COc1ccc2c(c1)c(c[nH]2)CN[C@H]3CCCC[C@H]3Nc4nc5ccccc5n4C</chem> $3\text{CF}_3\text{CO}_2\text{H}$	445.4 (M + H)	2.96
3324	 <chem>Oc1cc(Br)cc(Cl)c1CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.11
3325	 <chem>CC(C)Oc1ccc(cc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.17
3326	 <chem>FC(F)(F)S[C@@H](c1ccccc1)CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.27
3327	 <chem>COc1cc(Br)cc(OC)c1CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	514.4 (M + H)	3.07
3328	 <chem>Fc1cc(C(F)(F)F)ccc1CN[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	2.99

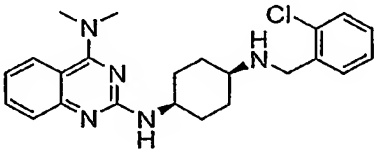
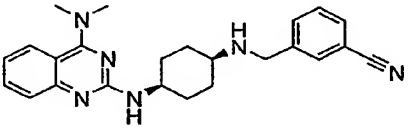
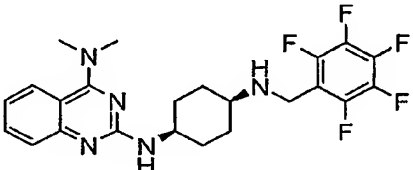
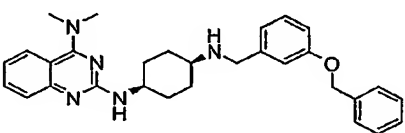
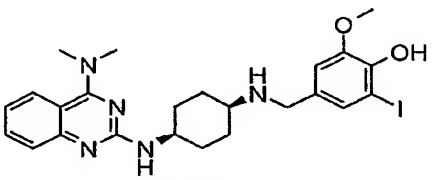
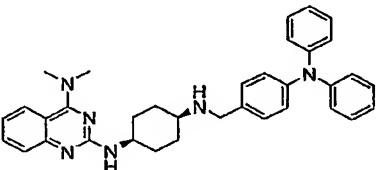
Example No.	Structure	ESI-MS	Retention Time (min)
3329	 $2\text{CF}_3\text{CO}_2\text{H}$	433.2 (M + H)	2.63
3330	 $2\text{CF}_3\text{CO}_2\text{H}$	518.4 (M + H)	3.63
3331	 $2\text{CF}_3\text{CO}_2\text{H}$	500.4 (M + H)	3.09
3332	 $3\text{CF}_3\text{CO}_2\text{H}$	379.4 (M + H)	2.77
3333	 $2\text{CF}_3\text{CO}_2\text{H}$	460.2 (M + H)	3.31
3334	 $2\text{CF}_3\text{CO}_2\text{H}$	512.4 (M + H)	3.51


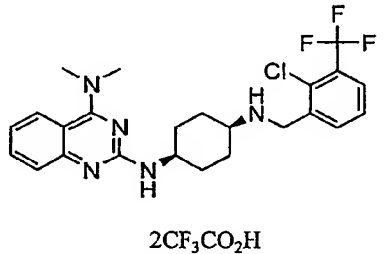
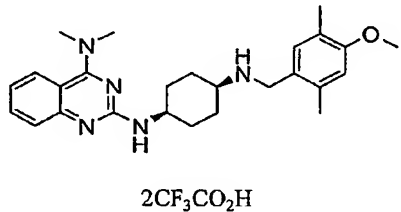
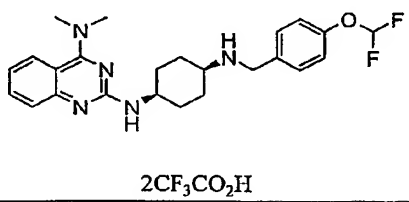
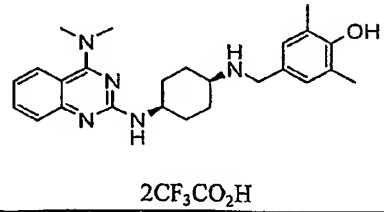
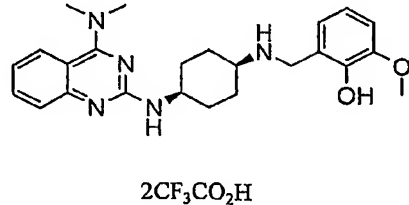
Example No.	Structure	ESI-MS	Retention Time (min)
3335	 2CF ₃ CO ₂ H	512.6 (M + H)	3.51
3336	 2CF ₃ CO ₂ H	476.2 (M + H)	3.39
3337	 2CF ₃ CO ₂ H	448.4 (M + H)	3.42
3338	 2CF ₃ CO ₂ H	404.4 (M + H)	3.17
3339	 2CF ₃ CO ₂ H	444.4 (M + H)	3.13
3340	 2CF ₃ CO ₂ H	462.2 (M + H)	3.21

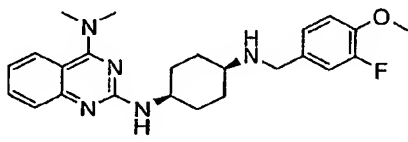
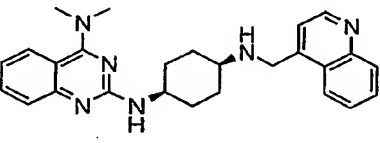
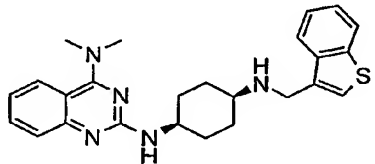
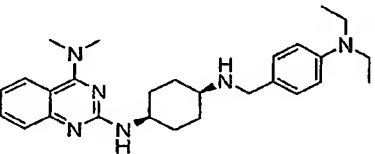
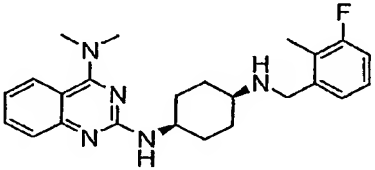
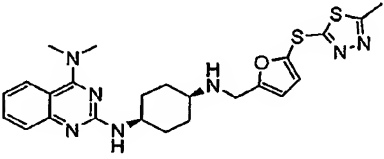
Example No.	Structure	ESI-MS	Retention Time (min)
3341	 $2\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	2.97
3342	 $2\text{CF}_3\text{CO}_2\text{H}$	444.6 (M + H)	3.16
3343	 $3\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	3.47
3344	 $2\text{CF}_3\text{CO}_2\text{H}$	456.4 (M + H)	3.47
3345	 $2\text{CF}_3\text{CO}_2\text{H}$	457.4 (M + H)	3.09
3346	 $2\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.37

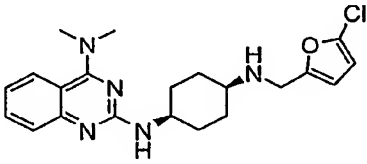
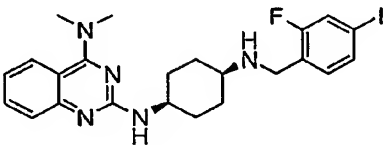
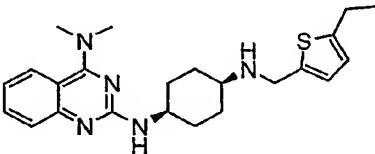
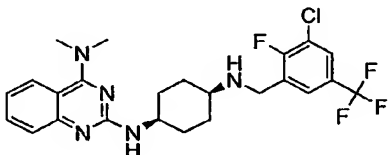
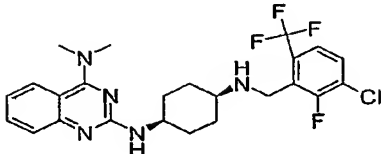
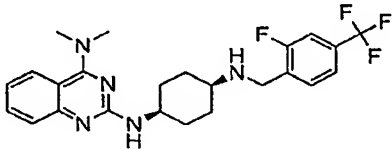
Example No.	Structure	ESI-MS	Retention Time (min)
3347	 <chem>COc1ccc(cc1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)CC2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.83
3348	 <chem>CCOC1=CC=C(C=C1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)CC2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30
3349	 <chem>CC(=O)OC1=CC(OC)=CC=C1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	494.4 (M + H)	2.98
3350	 <chem>OC1=CC=C(C=C1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)CC2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	406.4 (M + H)	2.80
3351	 <chem>FC(F)(F)Oc1ccc(cc1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)CC2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	3.20
3352	 <chem>Cc1ccc(cc1CN[C@H]2CCCC[C@H]2NC3=NC4=CC=CC=C4N(C)C3=NC5=CC=CC=C5)CC2</chem> $2\text{CF}_3\text{CO}_2\text{H}$	390.4 (M + H)	2.97

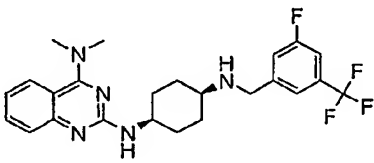
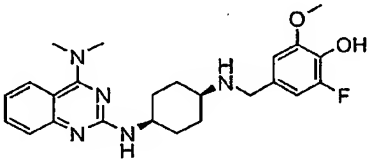
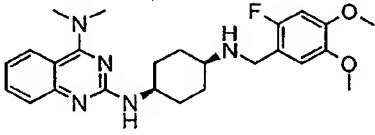
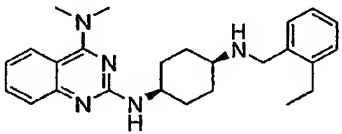
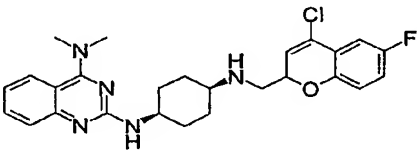
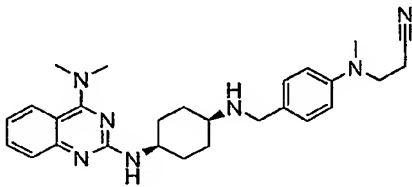
Example No.	Structure	ESI-MS	Retention Time (min)
3353	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CC=CC=C4Cl)cc5ccccc45</chem> $2\text{CF}_3\text{CO}_2\text{H}$	444.2 (M + H)	3.01
3354	 <chem>CN(C)c1nc2c(ncn2C1NCC3CCCCC3NCC4=CN=CN4)cc5ccccc45</chem> $3\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	2.27
3355	 <chem>CCN(CC)CCOCC1=CC=CC=C1NCC2CCCCC2NCC3=NC4=C(N(C)C)N=CN=C4C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	491.4 (M + H)	2.55
3356	 <chem>Clc1ccc(cc1)NCC2CCCCC2NCC3=NC4=C(N(C)C)N=CN=C4C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.05
3357	 <chem>COc1cccc(c1)NCC2CCCCC2NCC3=NC4=C(N(C)C)N=CN=C4C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	422.2 (M + H)	2.69
3358	 <chem>CC(C)Cc1ccc(cc1)NCC2CCCCC2NCC3=NC4=C(N(C)C)N=CN=C4C3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	3.36

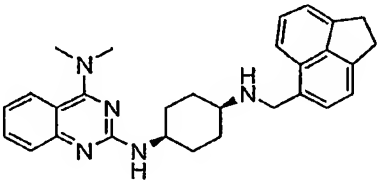
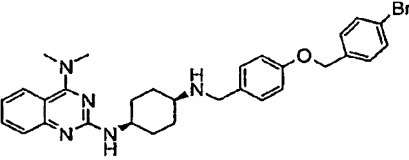
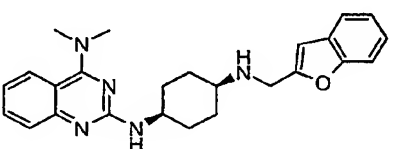
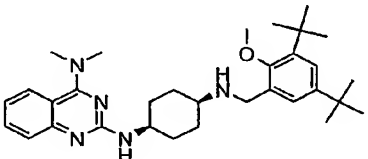
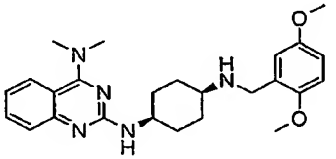
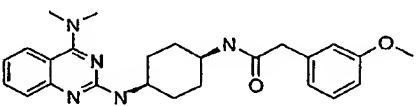
Example No.	Structure	ESI-MS	Retention Time (min)
3359	 $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	2.97
3360	 $2\text{CF}_3\text{CO}_2\text{H}$	401.2 (M + H)	2.81
3361	 $2\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.01
3362	 $2\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	3.43
3363	 $2\text{CF}_3\text{CO}_2\text{H}$	548.4 (M + H)	3.03
3364	 $3\text{CF}_3\text{CO}_2\text{H}$	543.6 (M + H)	3.95

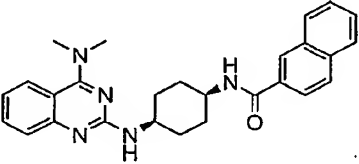
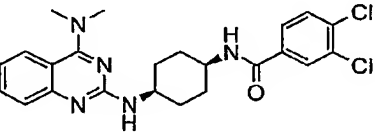
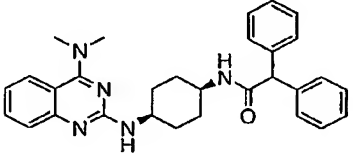
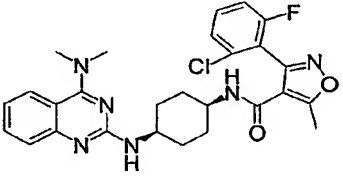
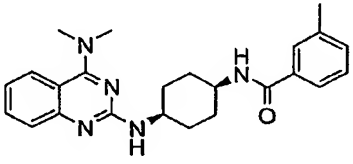
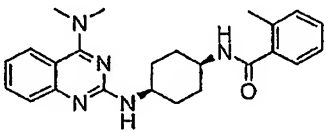
Example No.	Structure	ESI-MS	Retention Time (min)
3365	 2CF ₃ CO ₂ H	478.4 (M + H)	3.64
3366	 2CF ₃ CO ₂ H	478.4 (M + H)	3.29
3367	 2CF ₃ CO ₂ H	434.4 (M + H)	3.20
3368	 2CF ₃ CO ₂ H	442.4 (M + H)	3.09
3369	 2CF ₃ CO ₂ H	420.4 (M + H)	2.87
3370	 2CF ₃ CO ₂ H	422.2 (M + H)	2.79

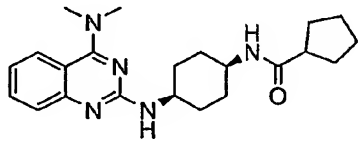
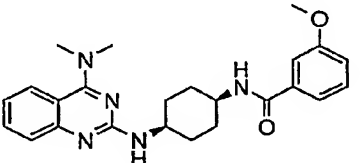
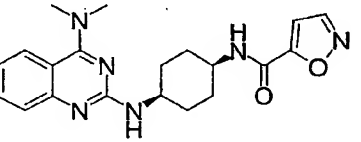
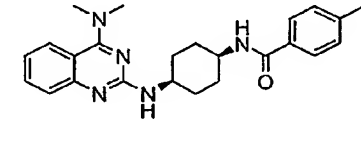
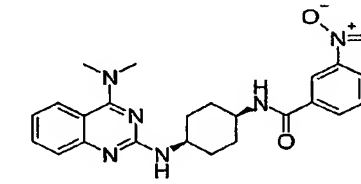
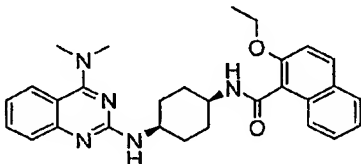
Example No.	Structure	ESI-MS	Retention Time (min)
3371	 2CF ₃ CO ₂ H	424.2 (M + H)	2.96
3372	 3CF ₃ CO ₂ H	427.2 (M + H)	2.53
3373	 2CF ₃ CO ₂ H	432.4 (M + H)	3.12
3374	 3CF ₃ CO ₂ H	447.4 (M + H)	2.45
3375	 2CF ₃ CO ₂ H	408.2 (M + H)	3.02
3376	 2CF ₃ CO ₂ H	496.4 (M + H)	2.81

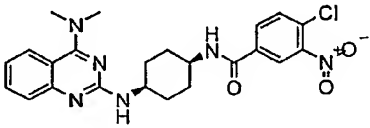
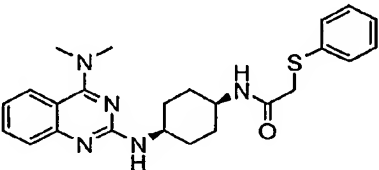
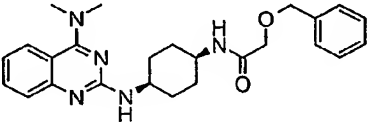
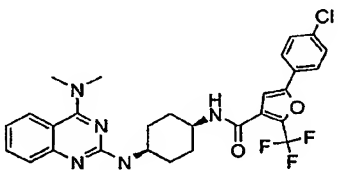
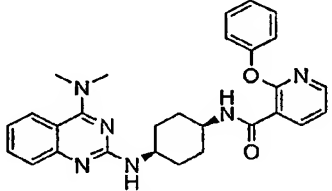
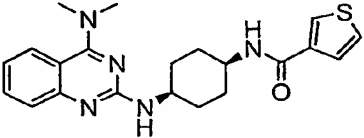
Example No.	Structure	ESI-MS	Retention Time (min)
3377	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4cc(Cl)ccc4)n1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	400.2 (M + H)	2.81
3378	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NCc4cc(I)ccc4F)n1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	520.2 (M + H)	3.14
3379	 <chem>CCc1cc(CSCC2CCCCC2NC3=NC4=CC=CC=C4N(C)C4=CN3)c(s1)</chem> $2\text{CF}_3\text{CO}_2\text{H}$	410.4 (M + H)	3.12
3380	 <chem>FC1=CC(=C(C(F)(F)F)C(F)=C1Cl)CCN2CCCCC2NC3=NC4=CC=CC=C4N(C)C4=CN3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.40
3381	 <chem>FC1=CC(=C(C(F)(F)F)C(F)=C1Cl)CCN2CCCCC2NC3=NC4=CC=CC=C4N(C)C4=CN3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	496.4 (M + H)	3.17
3382	 <chem>FC1=CC(=C(C(F)(F)F)C(F)=C1)CCN2CCCCC2NC3=NC4=CC=CC=C4N(C)C4=CN3</chem> $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.19

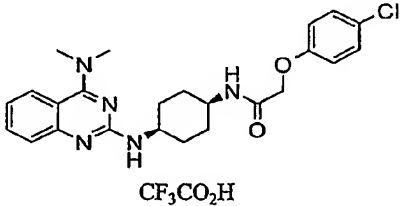
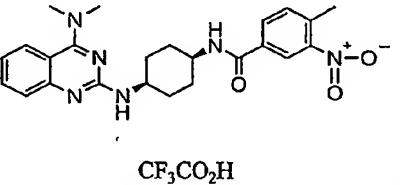
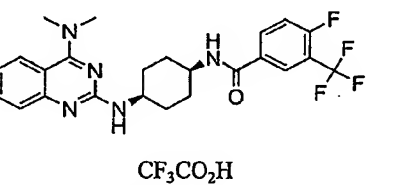
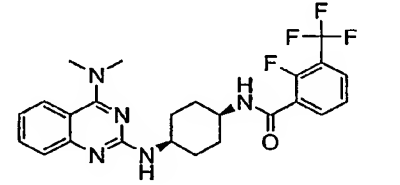
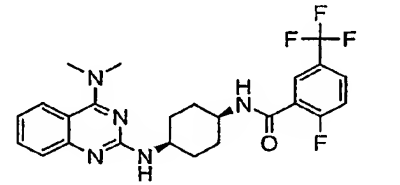
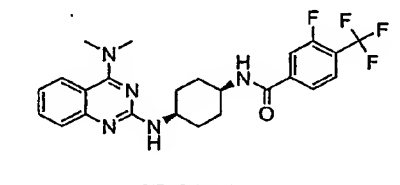
Example No.	Structure	ESI-MS	Retention Time (min)
3383	 $2\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	3.28
3384	 $2\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	2.74
3385	 $2\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	2.89
3386	 $2\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.09
3387	 $2\text{CF}_3\text{CO}_2\text{H}$	482.2 (M + H)	3.29
3388	 $3\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	2.99

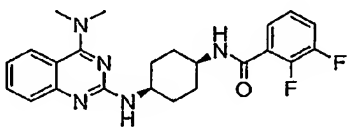
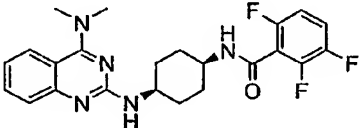
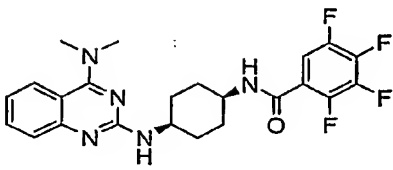
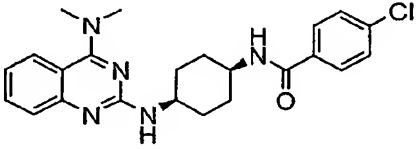
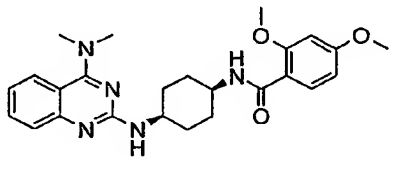
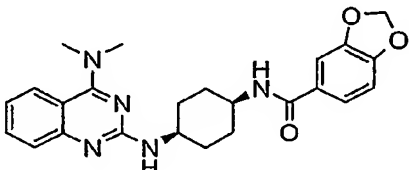
Example No.	Structure	ESI-MS	Retention Time (min)
3389	 $2\text{CF}_3\text{CO}_2\text{H}$	452.2 (M + H)	3.40
3390	 $2\text{CF}_3\text{CO}_2\text{H}$	560.2 (M + H)	3.73
3391	 $2\text{CF}_3\text{CO}_2\text{H}$	416.4 (M + H)	2.99
3392	 $2\text{CF}_3\text{CO}_2\text{H}$	518.6 (M + H)	4.08
3393	 $2\text{CF}_3\text{CO}_2\text{H}$	436.4 (M + H)	2.95
3394	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.30

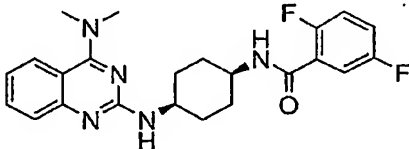
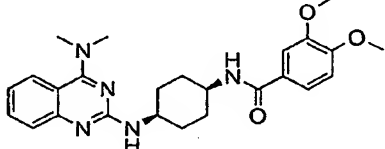
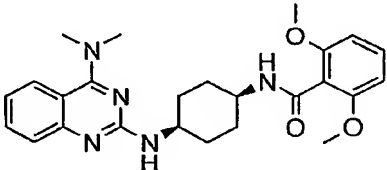
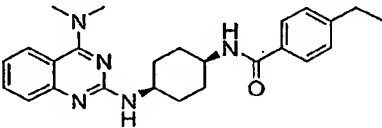
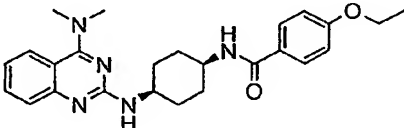
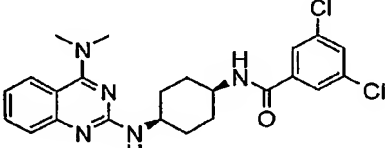
Example No:	Structure	ESI-MS	Retention Time (min)
3395	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.26
3396	 <chem>Clc1cc(Cl)ccc1C(=O)N[C@H]2CCCC[C@H]2N[C@@H]3C4=NC5=CC=CC=C5N(C)C4=NC3=CC=C3</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.39
3397	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)C(c4ccccc4)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	4.37
3398	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)N4C(=O)C(C)=C(F)C(Cl)=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	523.6 (M + H)	4.15
3399	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.46
3400	 <chem>CC1=NC2=CC=CC=C2N(C)C1N[C@H]3CCCC[C@H]3NC(=O)c4cc(C)ccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.75

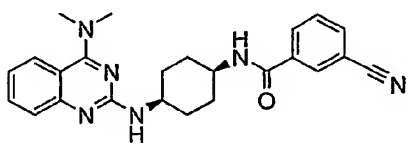
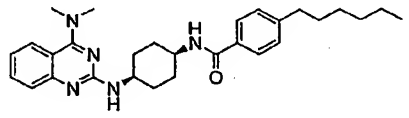
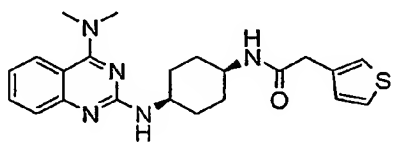
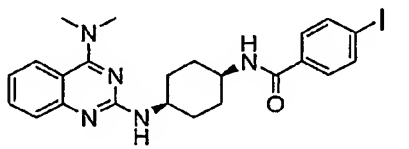
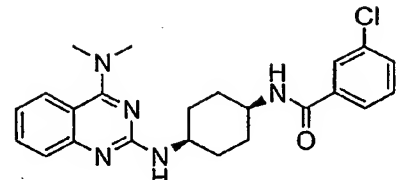
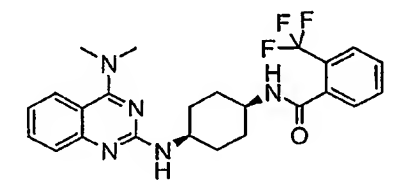
Example No.	Structure	ESI-MS	Retention Time (min)
3401	 <chem>CC1=CN(C)C(=N1)N[C@H]2CCCC[C@H]2NC(=O)C3CCCC3</chem> $\text{CF}_3\text{CO}_2\text{H}$	382.4 (M + H)	3.65
3402	 <chem>COc1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	3.81
3403	 <chem>Cc1cc2ocn2c(=O)[nH]1[C@H]3CCCC[C@H]3Nc4nc5ccccc5n4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	381.2 (M + H)	3.33
3404	 <chem>CC1=CN(C)C(=N1)N[C@H]2CCCC[C@H]2NC(=O)c3ccc(C)cc3</chem> $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	3.93
3405	 <chem>[O-][N+](=O)c1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	435.2 (M + H)	3.40
3406	 <chem>COc1ccc2cc(C(=O)N[C@H]3CCCC[C@H]3Nc4nc5ccccc5n4C)ccc2c1</chem> $\text{CF}_3\text{CO}_2\text{H}$	484.4 (M + H)	4.15

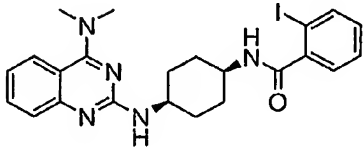
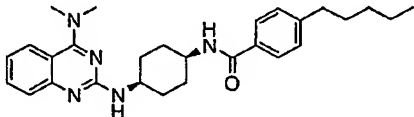
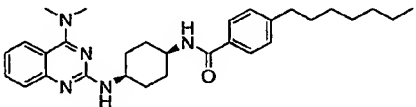
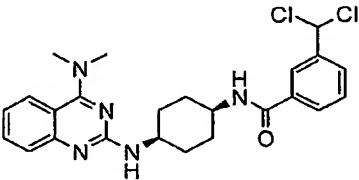
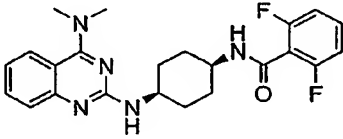
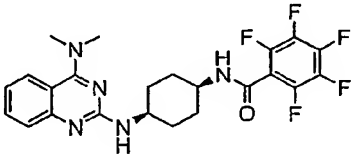
Example No.	Structure	ESI-MS	Retention Time (min)
3407	 $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.20
3408	 $\text{CF}_3\text{CO}_2\text{H}$	436.2 (M + H)	3.88
3409	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	3.91
3410	 $\text{CF}_3\text{CO}_2\text{H}$	558.4 (M + H)	4.92
3411	 $2\text{CF}_3\text{CO}_2\text{H}$	483.4 (M + H)	4.08
3412	 $\text{CF}_3\text{CO}_2\text{H}$	396.2 (M + H)	3.68

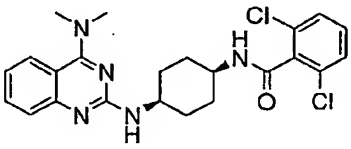
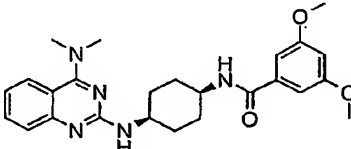
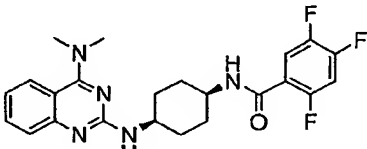
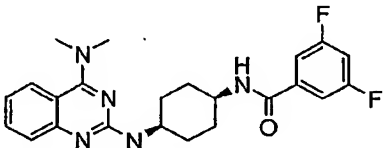
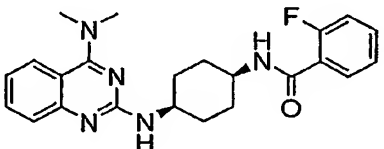
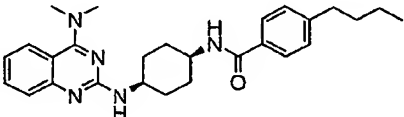
Example No.	Structure	ESI-MS	Retention Time (min)
3413	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)OCC4=CC=C(C=C4)Cl)C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	454.2 (M + H)	3.70
3414	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)Nc4ccc(cc4)[N+](=O)[O-])C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	449.4 (M + H)	4.09
3415	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)Nc4ccc(cc4)C(F)(F)F)C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.33
3416	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)Nc4ccccc4C(F)(F)F)C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	3.60
3417	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)Nc4ccccc4C(F)(F)F)C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.23
3418	 <chem>CN(C)c1nc2c(ncn2C1NC3CCCCC3NC(=O)Nc4ccc(cc4)C(F)(F)F)C5=CC=CC=C5.[CF3][O-]C(=O)O</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.4 (M + H)	4.38

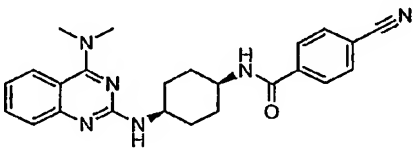
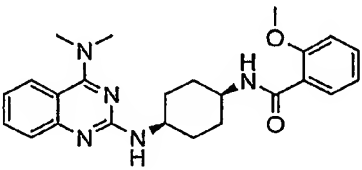
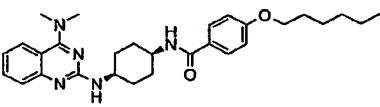
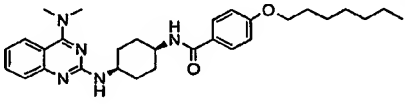
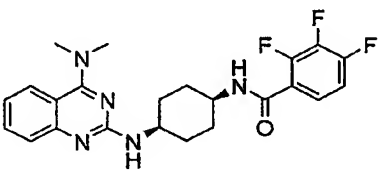
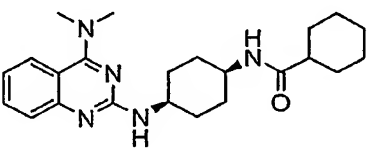
Example No.	Structure	ESI-MS	Retention Time (min)
3419	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC=C(C=C7)C(F)=C(F)C7</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.87
3420	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC(=CC=C7)C(F)=C(F)C7</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	3.86
3421	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC(=CC=C7)C(F)=C(F)C7</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.15
3422	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC=C(C=C7)C(Cl)=C7</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	4.06
3423	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC(=CC=C7)OC(=C7)OC7</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	4.03
3424	 <chem>CC1=NC2=CC=CC=C2N1N(C)C3=CC=CC=C3N3C4=CC=CC=C4C5=CC(=CC=C5)C(=O)N[C@H]6CCCC[C@H]6C7=CC=CC=C7OC7</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.2 (M + H)	3.75

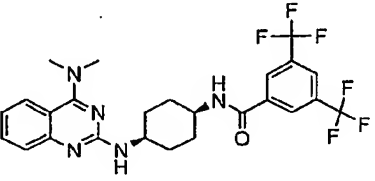
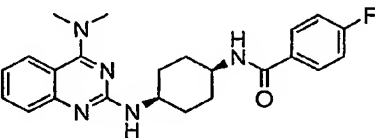
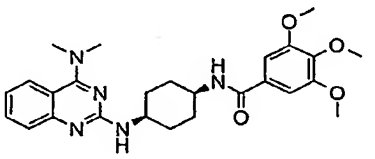
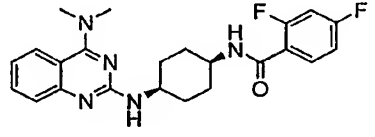
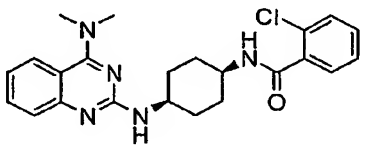
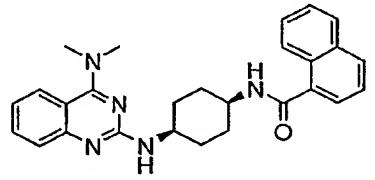
Example No.	Structure	ESI-MS	Retention Time (min)
3425	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4cc(F)cc(F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.88
3426	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4cc(OC)c(OC)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.64
3427	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4cc(OC)c(O)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.55
3428	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4ccc(CC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	418.6 (M + H)	4.17
3429	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4ccc(OCC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.03
3430	 <chem>CC1=NC2=CC=CC=C2N1C(=N)N(C)C3CCCC[C@H]3NC(=O)c4cc(Cl)c(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.45

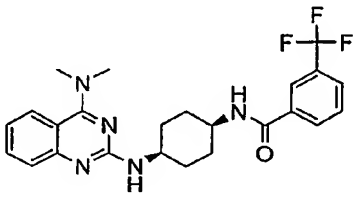
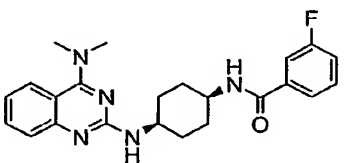
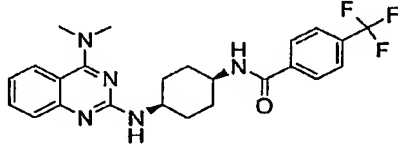
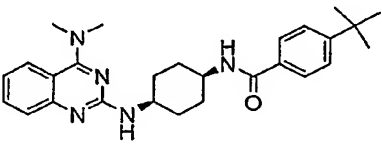
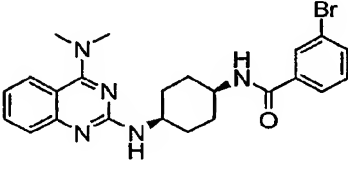
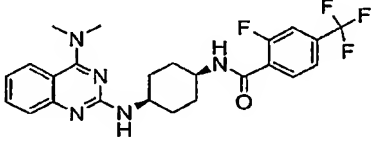
Example No.	Structure	ESI-MS	Retention Time (min)
3431	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3C(=O)Nc4ccc(C#N)cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	415.4 (M + H)	3.76
3432	 <chem>CCCCC(=O)c1ccc(cc1)C(=O)N[C@H]2CCCC[C@H]2Nc3nc4c(ncn3C)ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	5.06
3433	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3C(=O)NCCc4ccsc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	410.2 (M + H)	3.64
3434	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3C(=O)Nc4ccc(I)cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.2 (M + H)	4.24
3435	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3C(=O)Nc4ccc(Cl)cc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	4.09
3436	 <chem>CC1=NC2=CC=CC=C2N=C(NC3CCCCC3C(=O)NCCc4cc(C(F)(F)F)ccc4)N1</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	3.89

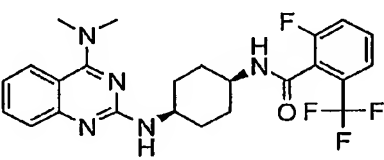
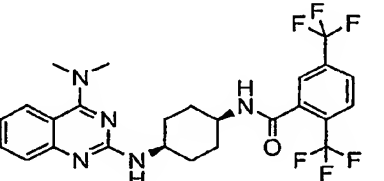
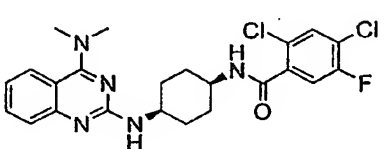
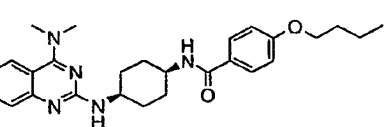
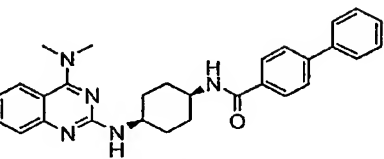
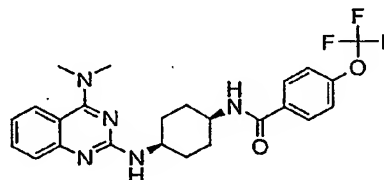
Example No.	Structure	ESI-MS	Retention Time (min)
3437	 CF ₃ CO ₂ H	516.2 (M + H)	3.88
3438	 CF ₃ CO ₂ H	460.4 (M + H)	4.86
3439	 CF ₃ CO ₂ H	488.4 (M + H)	4.70
3440	 CF ₃ CO ₂ H	472.4 (M + H)	4.29
3441	 CF ₃ CO ₂ H	426.2 (M + H)	3.69
3442	 CF ₃ CO ₂ H	480.2 (M + H)	4.16

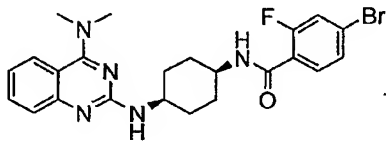
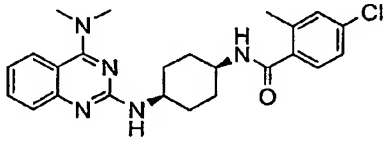
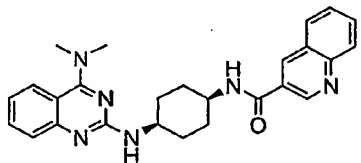
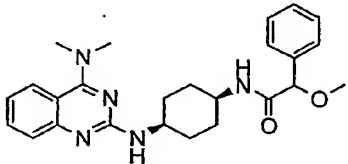
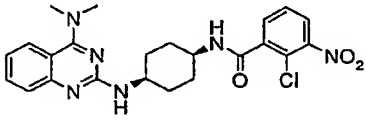
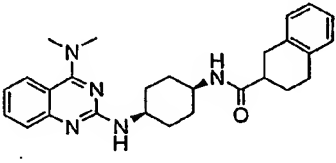
Example No.	Structure	ESI-MS	Retention Time (min)
3443	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@H]4CCCC[C@H]4NC(=O)c5cc(Cl)cc(Cl)c5</chem> <chem>CF3CO2H</chem>	458.2 (M + H)	3.91
3444	 <chem>COc1cc(OC)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3cc4c(cc3)N(C)N4)c1</chem> <chem>CF3CO2H</chem>	450.4 (M + H)	3.95
3445	 <chem>Fc1cc(F)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3cc4c(cc3)N(C)N4)c1</chem> <chem>CF3CO2H</chem>	444.4 (M + H)	4.01
3446	 <chem>Fc1cc(F)cc(C(=O)N[C@H]2CCCC[C@H]2Nc3cc4c(cc3)N(C)N4)c1</chem> <chem>CF3CO2H</chem>	426.2 (M + H)	4.00
3447	 <chem>Fc1ccccc1C(=O)N[C@H]2CCCC[C@H]2Nc3cc4c(cc3)N(C)N4</chem> <chem>CF3CO2H</chem>	408.4 (M + H)	3.75
3448	 <chem>CCCC1=CC=C(C=C1)C(=O)N[C@H]2CCCC[C@H]2Nc3cc4c(cc3)N(C)N4</chem> <chem>CF3CO2H</chem>	446.6 (M + H)	4.65

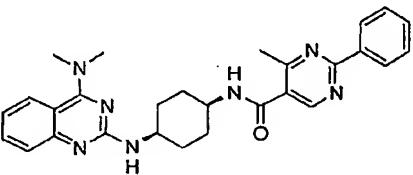
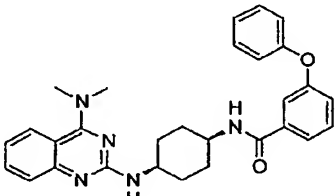
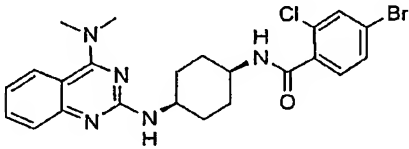
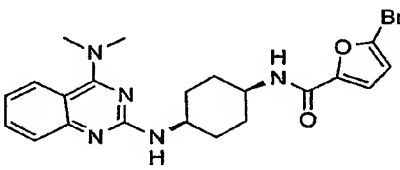
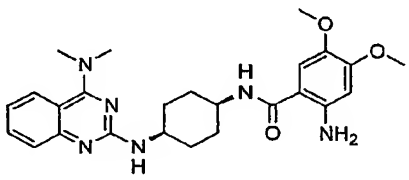
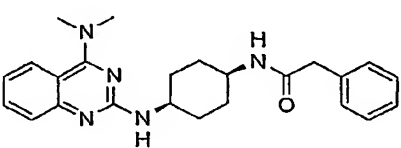
Example No.	Structure	ESI-MS	Retention Time (min)
3449	 CF ₃ CO ₂ H	415.2 (M + H)	3.75
3450	 CF ₃ CO ₂ H	420.4 (M + H)	3.91
3451	 CF ₃ CO ₂ H	490.4 (M + H)	4.99
3452	 CF ₃ CO ₂ H	504.4 (M + H)	5.16
3453	 CF ₃ CO ₂ H	444.4 (M + H)	4.00
3454	 CF ₃ CO ₂ H	396.2 (M + H)	3.85

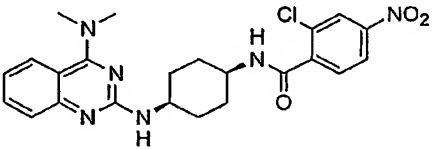
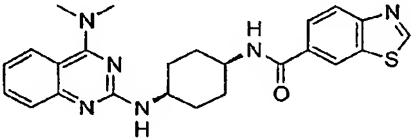
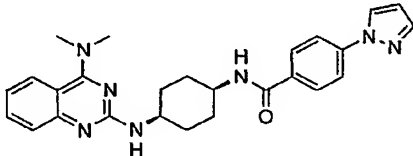
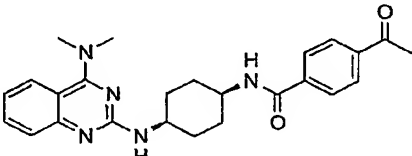
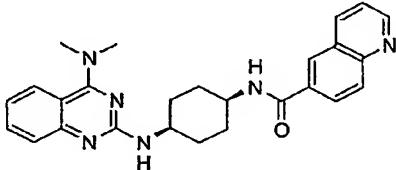
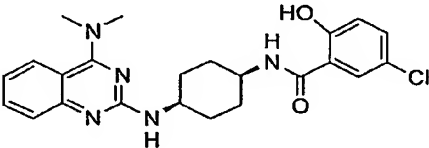
Example No.	Structure	ESI-MS	Retention Time (min)
3455	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC(=CC(=C5)C(F)(F)F)C(F)(F)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.6 (M + H)	4.69
3456	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC=C(C=C5)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.4 (M + H)	3.30
3457	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC(=CC(=C5)OC)OC)OC</chem> $\text{CF}_3\text{CO}_2\text{H}$	480.4 (M + H)	3.76
3458	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC(=CC(=C5)F)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	426.2 (M + H)	3.86
3459	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC=C(C=C5)Cl)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	424.2 (M + H)	3.76
3460	 <chem>CC1=NC2=CC=CC=C2N1N=C3C(=NC(=C3)N[C@@H]4CCCC[C@H]4NC(=O)C5=CC6=CC=CC=C6C5=C6</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.4 (M + H)	4.05

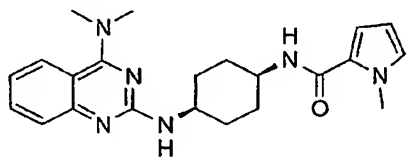
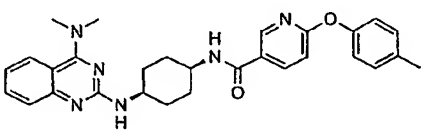
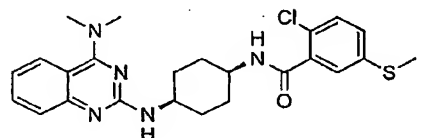
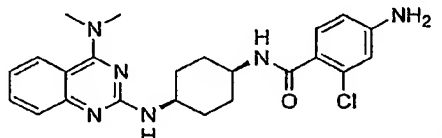
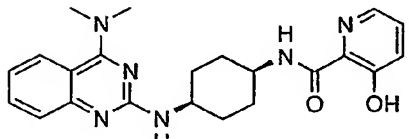
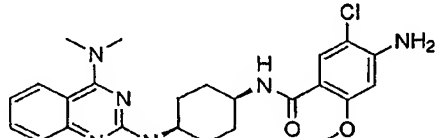
Example No.	Structure	ESI-MS	Retention Time (min)
3461	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5ccc(cc5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.4 (M + H)	4.25
3462	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5ccc(cc5)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	408.2 (M + H)	3.84
3463	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5ccc(cc5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.25
3464	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5ccc(cc5)C(C)(C)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	446.6 (M + H)	4.44
3465	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5ccc(cc5)Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	4.13
3466	 <chem>CC1(C)N2C=NC3C(=N1)N(C2)C3N[C@H]4CCCC[C@H]4NC(=O)c5cc(F)c(cc5)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.25

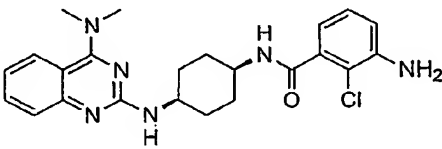
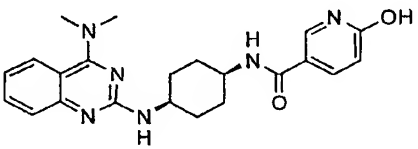
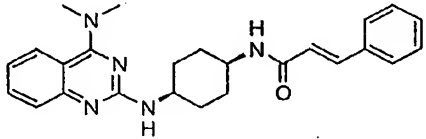
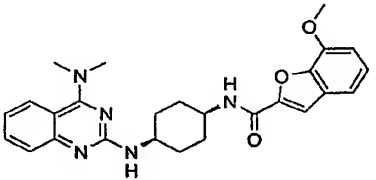
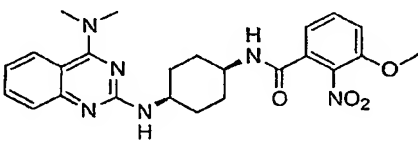
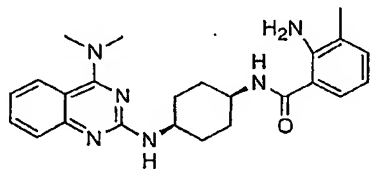
Example No.	Structure	ESI-MS	Retention Time (min)
3467	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC=C(C=C4)C(F)=C(C(F)(F)F)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.92
3468	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC(=CC=C4)C(F)(F)=C(C(F)(F)F)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	526.4 (M + H)	4.31
3469	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC(=CC=C4)C(F)=CC=C4Cl)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	4.15
3470	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC=C(C=C4)OCC)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	462.2 (M + H)	4.48
3471	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC=C(C=C4)C5=CC=CC=C5C6=CC=CC=C6)C7</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	4.45
3472	 <chem>CC1=NC2=CC=CC=C2N1N=C(NC3CCCCC3NC(=O)C4=CC=C(C=C4)OC(F)(F)F)C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.29

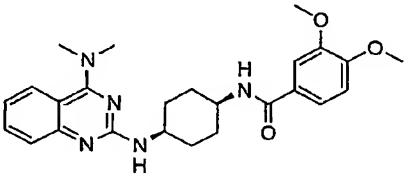
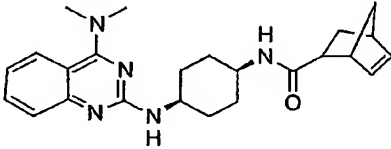
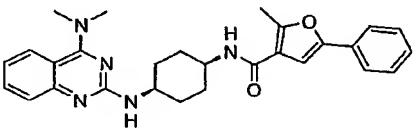
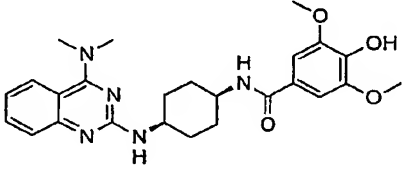
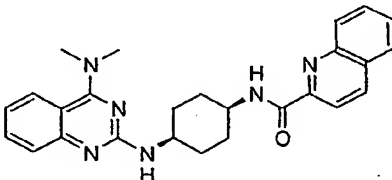
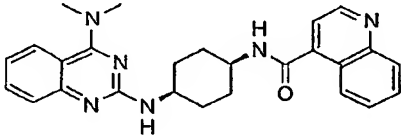
Example No.	Structure	ESI-MS	Retention Time (min)
3473	 $\text{CF}_3\text{CO}_2\text{H}$	486.2 (M + H)	4.32
3474	 $\text{CF}_3\text{CO}_2\text{H}$	438.4 (M + H)	4.31
3475	 $2\text{CF}_3\text{CO}_2\text{H}$	441.4 (M + H)	3.75
3476	 $\text{CF}_3\text{CO}_2\text{H}$	434.4 (M + H)	4.10
3477	 $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.19
3478	 $\text{CF}_3\text{CO}_2\text{H}$	444.4 (M + H)	4.36

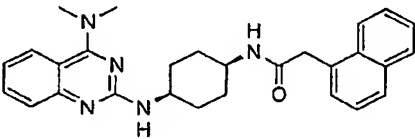
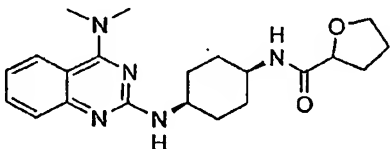
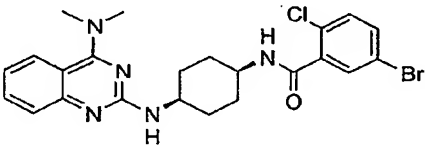
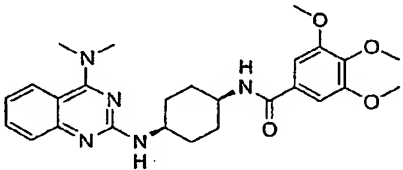
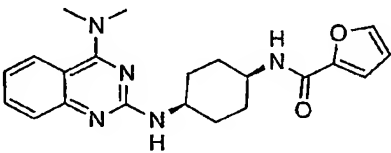
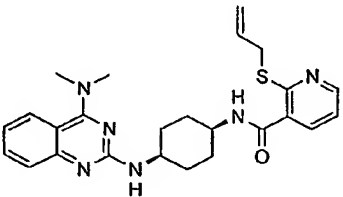
Example No.	Structure	ESI-MS	Retention Time (min)
3479	 $3\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.35
3480	 $\text{CF}_3\text{CO}_2\text{H}$	482.4 (M + H)	4.64
3481	 $\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	4.37
3482	 $\text{CF}_3\text{CO}_2\text{H}$	458.2 (M + H)	4.08
3483	 $2\text{CF}_3\text{CO}_2\text{H}$	465.4 (M + H)	3.66
3484	 $\text{CF}_3\text{CO}_2\text{H}$	404.4 (M + H)	4.03

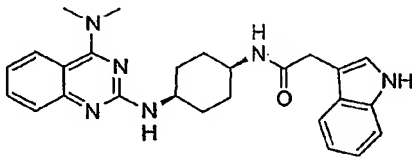
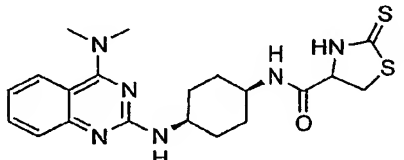
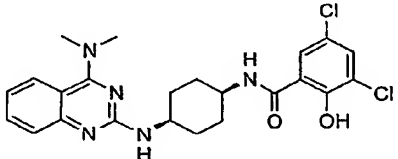
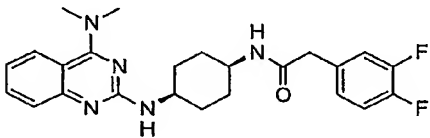
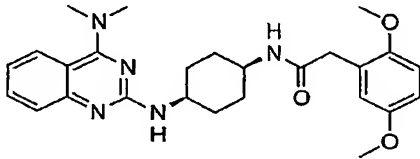
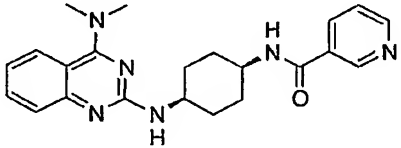
Example No.	Structure	ESI-MS	Retention Time (min)
3485	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC=C(C=C5)C(=O)C6=CC=CC=C6C7=CC=CC=C7[N+](=O)[O-]Cl</chem> $\text{CF}_3\text{CO}_2\text{H}$	469.4 (M + H)	4.23
3486	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC6=CC=CC=C6N7C8=CC=CC=C8S8=N7</chem> $2\text{CF}_3\text{CO}_2\text{H}$	447.4 (M + H)	3.94
3487	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC=C(C=C5)C(=O)C6=CC=CC=C6N7C8=CC=CC=C8N7</chem> $2\text{CF}_3\text{CO}_2\text{H}$	456.2 (M + H)	4.07
3488	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC=C(C=C5)C(=O)C6=CC=CC=C6C(=O)C</chem> $\text{CF}_3\text{CO}_2\text{H}$	432.4 (M + H)	3.99
3489	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC6=CC=CC=C6N7C8=CC=CC=C8N7</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.3 (M + H)	1.70
3490	 <chem>CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3N4CCCCC4NC(=O)C5=CC=C(C=C5)C(=O)C6=CC=CC=C6C7=CC=CC=C7OCl</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.2 (M + H)	4.57

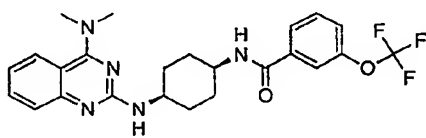
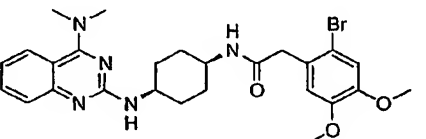
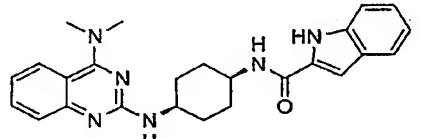
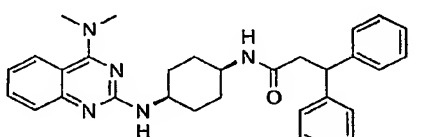
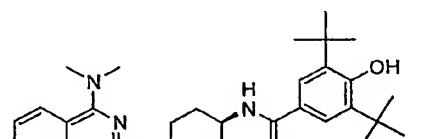
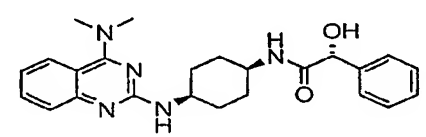
Example No.	Structure	ESI-MS	Retention Time (min)
3491	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc[nH]4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	393.4 (M + H)	4.01
3492	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(Oc5ccc(O)cc5)cc4)c5ccccc15</chem> $2\text{CF}_3\text{CO}_2\text{H}$	497.4 (M + H)	4.45
3493	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4ccc(Cl)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.2 (M + H)	2.40
3494	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(N)cc(Cl)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.92
3495	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(O)ccn4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	2.30
3496	 <chem>CN(C)c1nc2c(ncn2C3CCCCC3NC(=O)c4cc(N)cc(Cl)c4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	469.5 (M + H)	2.27

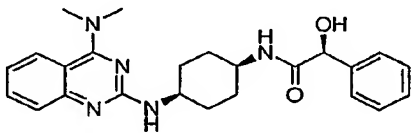
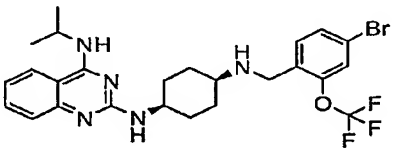
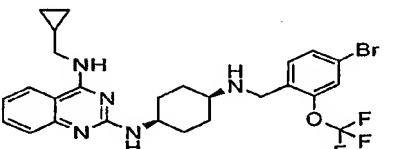
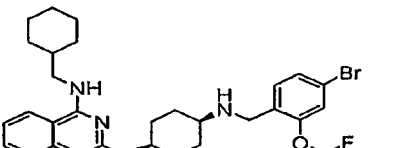
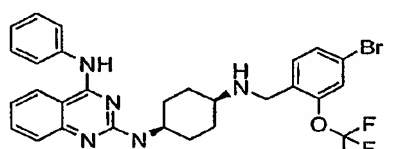
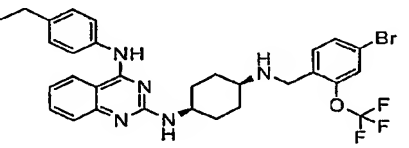
Example No.	Structure	ESI-MS	Retention Time (min)
3497	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)c4cc(N)ccc4Cl</chem> $2\text{CF}_3\text{CO}_2\text{H}$	439.4 (M + H)	1.93
3498	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)c4cc(O)nc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	407.4 (M + H)	1.62
3499	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)/C=C/c4ccccc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	416.3 (M + H)	2.34
3500	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)c4cc(OC)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	460.4 (M + H)	2.46
3501	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)c4cc(OC)c([N+](=O)[O-])cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	465.4 (M + H)	4.13
3502	 <chem>CN1C=NC2=C(N1)C=CC=C2N3CCCCC3NC(=O)c4cc(N)ccc4</chem> $2\text{CF}_3\text{CO}_2\text{H}$	419.4 (M + H)	3.87

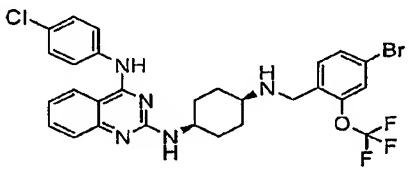
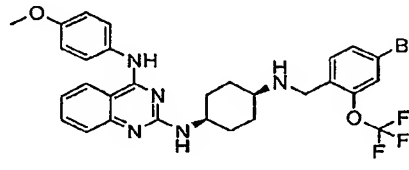
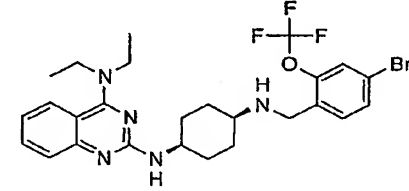
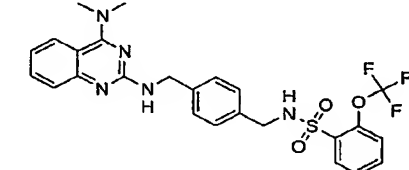
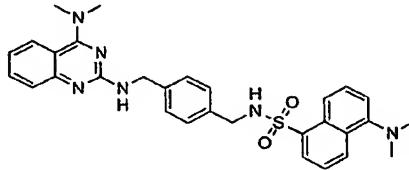
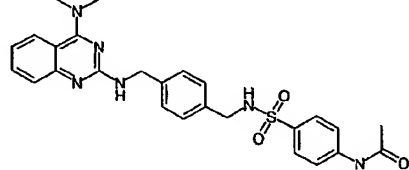
Example No.	Structure	ESI-MS	Retention Time (min)
3503	 <chem>COc1ccc(cc1)C(=O)Nc2ccc(cc2)Nc3nc(C)c(C)n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	3.97
3504	 <chem>C1CC2C(C1)C(=O)Nc3ccc(cc3)Nc4nc(C)c(C)n4</chem> $\text{CF}_3\text{CO}_2\text{H}$	406.2 (M + H)	2.18
3505	 <chem>Cc1cc2ccccc2o1C(=O)Nc3ccc(cc3)Nc4nc(C)c(C)n4</chem> $\text{CF}_3\text{CO}_2\text{H}$	470.4 (M + H)	4.74
3506	 <chem>COc1cc(O)cc(OC)c1C(=O)Nc2ccc(cc2)Nc3nc(C)c(C)n3</chem> $\text{CF}_3\text{CO}_2\text{H}$	466.4 (M + H)	3.83
3507	 <chem>c1ccc2nc3ccc(cc3n2)C(=O)Nc4ccc(cc4)Nc5nc(C)c(C)n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	4.38
3508	 <chem>c1ccc2nc3ccc(cc3n2)C(=O)Nc4ccc(cc4)Nc5nc(C)c(C)n5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	441.2 (M + H)	3.62

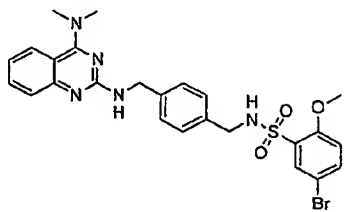
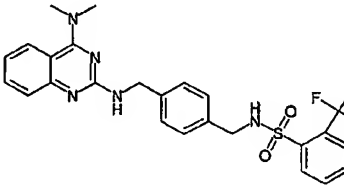
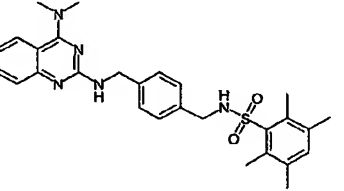
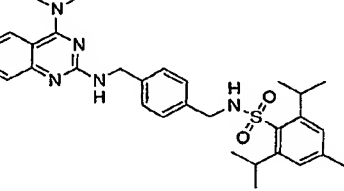
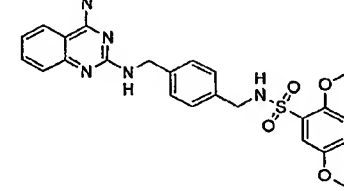
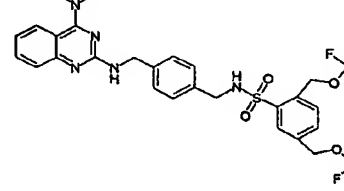
Example No.	Structure	ESI-MS	Retention Time (min)
3509	 $\text{CF}_3\text{CO}_2\text{H}$	454.5 (M + H)	2.44
3510	 $\text{CF}_3\text{CO}_2\text{H}$	384.4 (M + H)	3.67
3511	 $\text{CF}_3\text{CO}_2\text{H}$	502.2 (M + H)	4.37
3512	 $\text{CF}_3\text{CO}_2\text{H}$	480.5 (M + H)	2.18
3513	 $\text{CF}_3\text{CO}_2\text{H}$	380.2 (M + H)	3.81
3514	 $2\text{CF}_3\text{CO}_2\text{H}$	463.2 (M + H)	4.23

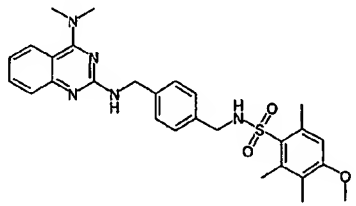
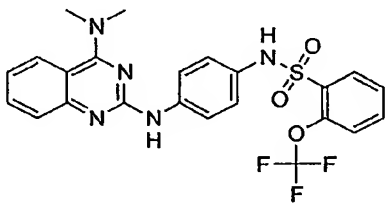
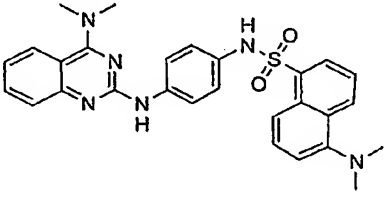
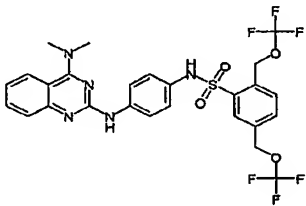
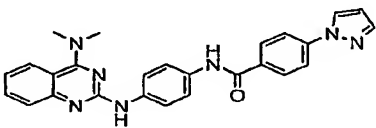
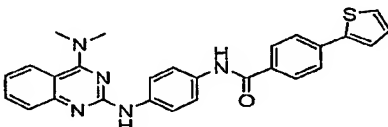
Example No.	Structure	ESI-MS	Retention Time (min)
3515	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5c[nH]c6ccccc56</chem> $2\text{CF}_3\text{CO}_2\text{H}$	443.4 (M + H)	2.12
3516	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5c[nH]c6c(s)scc56</chem> $\text{CF}_3\text{CO}_2\text{H}$	431.1 (M + H)	1.90
3517	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5c(Cl)c(Cl)c(O)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	5.05
3518	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5cc(F)c(F)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	440.5 (M + H)	2.33
3519	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5cc(OC)c(OC)cc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.5 (M + H)	2.20
3520	 <chem>CC1=CN2C(=N1)N(C)C2c3ccccc3N[C@@H]4CCCC[C@H]4NC(=O)Cc5cccnc5</chem> $2\text{CF}_3\text{CO}_2\text{H}$	391.1 (M + H)	1.59

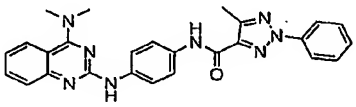
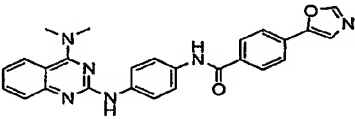
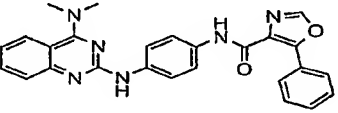
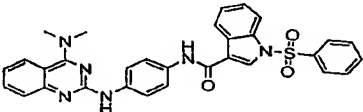
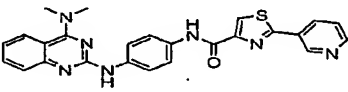
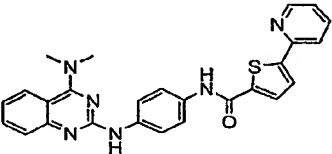
Example No.	Structure	ESI-MS	Retention Time (min)
3521	 $\text{CF}_3\text{CO}_2\text{H}$	474.4 (M + H)	4.53
3522	 $\text{CF}_3\text{CO}_2\text{H}$	542.2 (M + H)	2.26
3523	 $2\text{CF}_3\text{CO}_2\text{H}$	429.3 (M + H)	2.41
3524	 $\text{CF}_3\text{CO}_2\text{H}$	494.6 (M + H)	2.59
3525	 $\text{CF}_3\text{CO}_2\text{H}$	518.5 (M + H)	2.96
3526	 $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.19

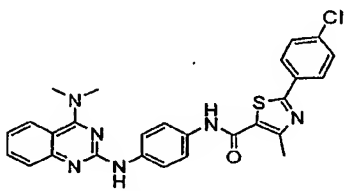
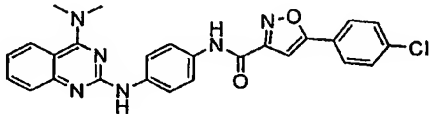
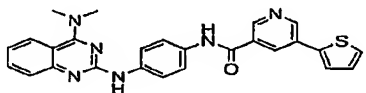
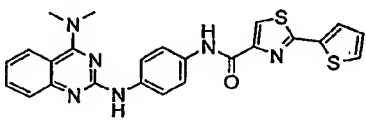
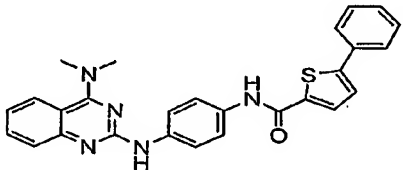
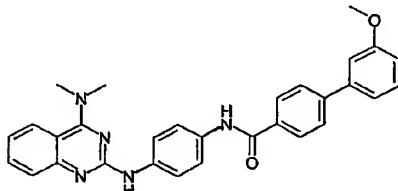
Example No.	Structure	ESI-MS	Retention Time (min)
3527	 <chem>CC1(C)Nc2nc3ccccc3n2N[C@H]4CCCC[C@H]4C(=O)C(O)c5ccccc5</chem> $\text{CF}_3\text{CO}_2\text{H}$	420.4 (M + H)	2.19
3528	 <chem>CC(C)Nc1nc2ccccc2n1N[C@H]3CCCC[C@H]3C(=O)C(O)c4cc(Br)ccc4OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	2.45
3529	 <chem>C1CC1Nc2nc3ccccc3n2N[C@H]4CCCC[C@H]4C(=O)C(O)c5cc(Br)ccc5OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	564.2 (M + H)	2.48
3530	 <chem>C1CCCCC1Nc2nc3ccccc3n2N[C@H]4CCCC[C@H]4C(=O)C(O)c5cc(Br)ccc5OC(F)(F)F</chem> $2\text{CF}_3\text{CO}_2\text{H}$	606.0 (M + H)	2.86
3531	 <chem>c1ccc(Nc2nc3ccccc3n2N[C@H]4CCCC[C@H]4C(=O)C(O)c5cc(Br)ccc5OC(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	586.2 (M + H)	3.20
3532	 <chem>CCc1ccc(Nc2nc3ccccc3n2N[C@H]4CCCC[C@H]4C(=O)C(O)c5cc(Br)ccc5OC(F)(F)F)cc1</chem> $2\text{CF}_3\text{CO}_2\text{H}$	614.4 (M + H)	2.76

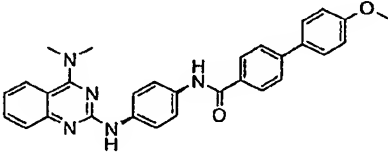
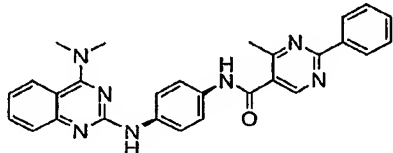
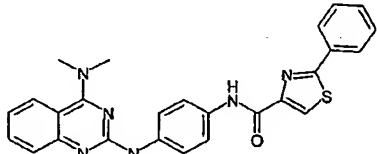
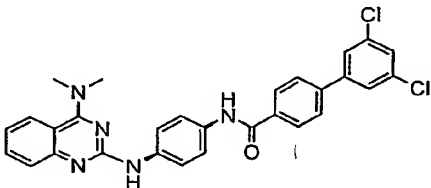
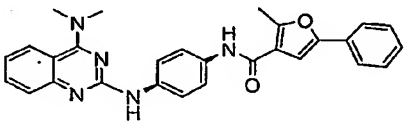
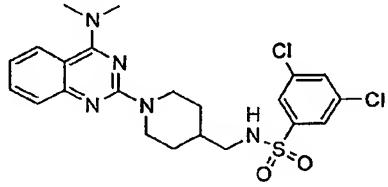
Example No.	Structure	ESI-MS	Retention Time (min)
3533	 $2\text{CF}_3\text{CO}_2\text{H}$	620.0 (M + H)	2.68
3534	 $2\text{CF}_3\text{CO}_2\text{H}$	616.0 (M + H)	2.56
3535	 $2\text{CF}_3\text{CO}_2\text{H}$	566.0 (M + H)	2.54
3536	 $\text{CF}_3\text{CO}_2\text{H}$	532.2 (M + H)	3.35
3537	 $2\text{CF}_3\text{CO}_2\text{H}$	541.4 (M + H)	3.11
3538	 $\text{CF}_3\text{CO}_2\text{H}$	505.2 (M + H)	2.98

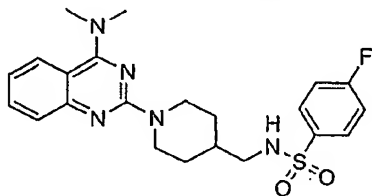
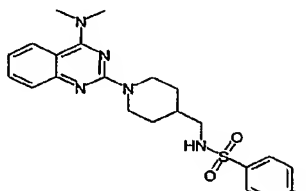
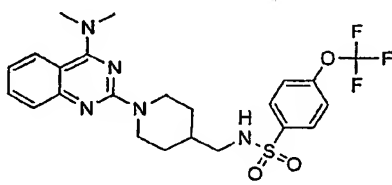
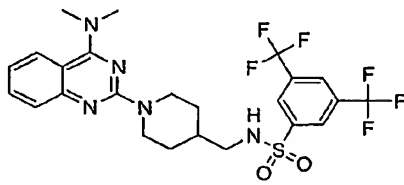
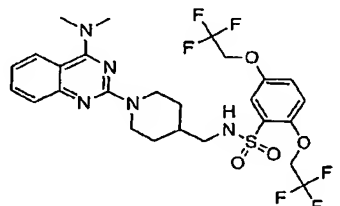
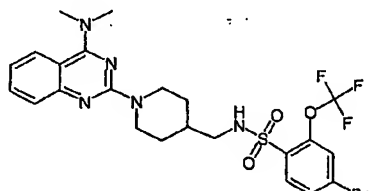
Example No.	Structure	ESI-MS	Retention Time (min)
3539	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=CC(=CC=C4)OC5=CC=CC=C5Br</chem> $\text{CF}_3\text{CO}_2\text{H}$	556 (M + H)	3.37
3540	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=CC=CC=C4C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	516.4 (M + H)	3.39
3541	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=C(C)C(C)=CC(C)=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	504.4 (M + H)	3.61
3542	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=C(C)C(C)=CC(C)=C4</chem> $\text{CF}_3\text{CO}_2\text{H}$	574.4 (M + H)	4.27
3543	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=CC(=CC=C4)OC5=CC(OC)=CC=C5</chem> $\text{CF}_3\text{CO}_2\text{H}$	508.2 (M + H)	3.17
3544	 <chem>CC1=NC2=CC=CC=C2N1N=CNC3=CC=CC=C3CS(=O)(=O)C4=CC(=CC=C4)COC(F)(F)F5=CC(OC(F)(F)F)=CC=C54</chem> $\text{CF}_3\text{CO}_2\text{H}$	644.2 (M + H)	3.63

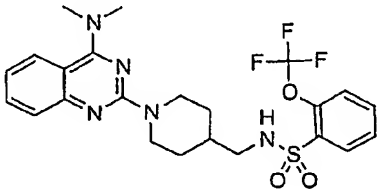
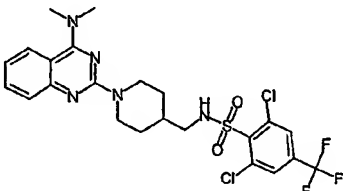
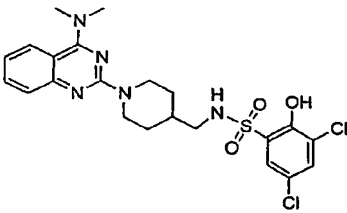
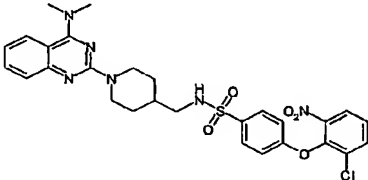
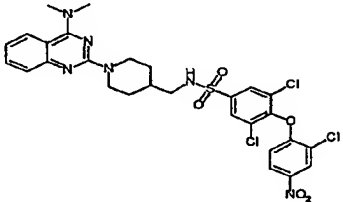
Example No.	Structure	ESI-MS	Retention Time (min)
3545	 $\text{CF}_3\text{CO}_2\text{H}$	520.4 (M + H)	3.56
3546	 $\text{CF}_3\text{CO}_2\text{H}$	504.2 (M + H)	3.25
3547	 $2\text{CF}_3\text{CO}_2\text{H}$	513.4 (M + H)	2.86
3548	 $\text{CF}_3\text{CO}_2\text{H}$	616.2 (M + H)	3.73
3549	 $2\text{CF}_3\text{CO}_2\text{H}$	450.4 (M + H)	2.79
3550	 $\text{CF}_3\text{CO}_2\text{H}$	466.2 (M + H)	3.35

Example No.	Structure	ESI-MS	Retention Time (min)
3551	 $2\text{CF}_3\text{CO}_2\text{H}$	465.2 (M + H)	3.34
3552	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	3.83
3553	 $\text{CF}_3\text{CO}_2\text{H}$	451.2 (M + H)	4.10
3554	 $\text{CF}_3\text{CO}_2\text{H}$	563.2 (M + H)	4.33
3555	 $2\text{CF}_3\text{CO}_2\text{H}$	468.4 (M + H)	3.66
3556	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	2.85

Example No.	Structure	ESI-MS	Retention Time (min)
3557	 $\text{CF}_3\text{CO}_2\text{H}$	515.4 (M + H)	3.52
3558	 $\text{CF}_3\text{CO}_2\text{H}$	485.2 (M + H)	3.40
3559	 $2\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.90
3560	 $\text{CF}_3\text{CO}_2\text{H}$	473.4 (M + H)	4.17
3561	 $\text{CF}_3\text{CO}_2\text{H}$	467.4 (M + H)	3.57
3562	 $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	4.00

Example No.	Structure	ESI-MS	Retention Time (min)
3563	 <chem>COc1ccc(cc1)C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	490.2 (M + H)	3.99
3564	 <chem>c1ccc(cc1)c2ccncc2C(=O)Nc3ccc(cc3)Nc4nc5ccccc5n4C</chem> $2\text{CF}_3\text{CO}_2\text{H}$	476.2 (M + H)	3.76
3565	 <chem>c1ccc(cc1)c2ccsc2C(=O)Nc3ccc(cc3)Nc4nc5ccccc5n4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	467.2 (M + H)	4.07
3566	 <chem>Clc1cc(Cl)ccc1C(=O)Nc2ccc(cc2)Nc3nc4ccccc4n3C</chem> $\text{CF}_3\text{CO}_2\text{H}$	528.2 (M + H)	4.53
3567	 <chem>c1ccc(cc1)c2ccoc2C(=O)Nc3ccc(cc3)Nc4nc5ccccc5n4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	464.2 (M + H)	4.11
3568	 <chem>Clc1cc(Cl)ccc1S(=O)(=O)NCc2ccncc2C3CCCCC3Nc4nc5ccccc5n4C</chem> $\text{CF}_3\text{CO}_2\text{H}$	494.0 (M + H)	3.43

Example No.	Structure	ESI-MS	Retention Time (min)
3569	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	444.0 (M + H)	3.03
3570	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(I)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	552.0 (M + H)	3.30
3571	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(OC(F)(F)F)cc4</chem> $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.37
3572	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(cc4-c5ccc(cc5)C(F)(F)F)C(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.66
3573	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4ccc(cc4-c5ccc(cc5)OC(F)(F)F)OC(F)(F)F</chem> $\text{CF}_3\text{CO}_2\text{H}$	622.0 (M + H)	3.61
3574	 <chem>CC1=NC2=C(N1)N=CN=C2CN3CCCCC3CNS(=O)(=O)c4cc(Br)cc(OC(F)(F)F)c4</chem> $\text{CF}_3\text{CO}_2\text{H}$	588.0 (M + H)	3.59

Example No.	Structure	ESI-MS	Retention Time (min)
3575	 $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.31
3576	 $\text{CF}_3\text{CO}_2\text{H}$	562.0 (M + H)	3.61
3577	 $\text{CF}_3\text{CO}_2\text{H}$	510.0 (M + H)	3.35
3578	 $\text{CF}_3\text{CO}_2\text{H}$	597.0 (M + H)	3.55
3579	 $\text{CF}_3\text{CO}_2\text{H}$	665.0 (M + H)	4.02

Assay Procedures

Compounds identified and disclosed throughout this patent document were assayed according to the protocols found in co-pending patent application having U.S. Serial Number 09/826,509, which is incorporated herein by reference.

Example 3580

Preparation of Endogenous MCH Receptor.

The endogenous human MCH receptor was obtained by PCR using genomic DNA as template and rTth polymerase (Perkin Elmer) with the buffer system provided by the manufacturer, 0.25 μ M of each primer, and 0.2 mM of each 4 nucleotides. The cycle condition was 30 cycles of 94°C for 1 min, 56°C for 1min and 72 °C for 1 min and 20 sec.

The 5' PCR primer contained a HindIII site with the sequence:

5'-GTGAAGCTTGCCCTCTGGTGCCTGCAGGAGG-3' (SEQ.ID.NO.:1)

and the 3' primer contained an EcoRI site with the sequence:

5'-GCAGAATTCCCGGTGGCGTGTGTGGTGCCC-3' (SEQ.ID.NO.:2).

The 1.3 kb PCR fragment was digested with HindIII and EcoRI and cloned into HindIII-EcoRI site of CMVp expression vector. Later the cloning work by Lakaye et al showed that there is an intron the coding region of the gene. Thus the 5' end of the cDNA was obtained by 5' RACE PCR using Clontech's marathon-ready hypothalamus cDNA as template and the manufacturer's recommended protocol for cycling condition. The 5' RACE PCR for the first and second round PCR were as follows:

5'-CATGAGCTGGTGGATCATGAAGGG-3' (SEQ.ID.NO.:3) and

5'-ATGAAGGGCATGCCAGGAGAAAG-3' (SEQ.ID.NO.:4).

Nucleic acid and amino acid sequences were thereafter determined and verified with the published sequences found on GenBank having Accession Number U71092.

Example 3581

Preparation of Non-Endogenous, Constitutively Active MCH Receptor.

Preparation of a non-endogenous version of the human MCH receptor was accomplished by creating a MCH-IC3-SST2 mutation (*see*; SEQ.ID.NO.:7 for nucleic acid sequence, and SEQ.ID.NO.:8 for amino acid sequence). Blast result showed that MCH receptor had the highest sequence homology to known SST2 receptor. Thus the third intracellular loop ("IC3") of MCH receptor was replaced with that of the IC3 of SST2

receptor to see if the chimera would show constitutive activity.

The BamHI-BstEII fragment containing IC3 of MCH receptor was replaced with synthetic oligonucleotides that contained the IC3 of SST2. The PCR sense mutagenesis primer used had the following sequence:

5'-GATCCTGCAGAAGGTGAAGTCCTCTGGAATCCGAGTGGGCTCCTCTAAGAG
GAAGAAGTCTGAGAAGAAG-3' (SEQ.ID.NO.:9)

and the antisense primer had the following sequence:

5'-GTGACCTTCTTCTCAGACTTCTTCTCTTAGAGGAGCCCACTCGGATTCCAG
AGGACTTCACCTTCTGCAG-3' (SEQ.ID.NO.:10).

The endogenous MCH receptor cDNA was used as a template.

Example 3582

GPCR Fusion Protein Preparation.

MCH Receptor-Gi α Fusion Protein construct was made as follows: primers were designed for endogenous MCH receptor was as follows:

5'-GTGAAGCTTGCCCGGGCAGGATGGACCTGG-3' (SEQ.ID.NO.:11; sense)

5'-ATCTAGAGGTGCCTTTGCTTTCTG-3' (SEQ.ID.NO.:12; anitsense).

The sense and anti-sense primers included the restriction sites for KB4 and XbaI, respectively.

PCR was utilized to secure the respective receptor sequences for fusion within the Gi α universal vector disclosed above, using the following protocol for each: 100ng cDNA for MCH receptor was added to separate tubes containing 2ul of each primer (sense and anti-sense), 3uL of 10mM dNTPs, 10uL of 10XTaqPlus™ Precision buffer, 1uL of TaqPlus™ Precision polymerase (Stratagene: #600211), and 80uL of water. Reaction temperatures and cycle times for MCH receptor were as follows: the initial denaturing step was done at 94°C for five minutes, and a cycle of 94°C for 30 seconds; 55°C for 30 seconds; 72°C for two minutes. A final extension time was done at 72°C for ten minutes. PCR product for was run on a 1% agarose gel and then purified (data not shown). The purified product was digested with KB4 and XbaI (New England Biolabs) and the desired inserts will be isolated, purified and ligated into the Gi universal vector at the respective restriction site. The positive clones was isolated following transformation and determined by restriction enzyme digest; expression using 293 cells was accomplished

following the protocol set forth *infra*. Each positive clone for MCH receptor: Gi-Fusion Protein was sequenced and made available for the direct identification of candidate compounds. (See, SEQ.ID.NO.:13 for nucleic acid sequence and SEQ.ID.NO.:14 for amino acid sequence).

Endogenous version of MCH receptor was fused upstream from the G protein Gi and is located at nucleotide 1 through 1,059 (see, SEQ.ID.NO.:13) and amino acid residue 1 through 353 (see, SEQ.ID.NO.:14). With respect to the MCH receptor, 2 amino acid residues (an equivalent of 6 nucleotides) were placed in between the endogenous (or non-endogenous) GPCR and the start codon for the G protein $G_{i\alpha}$. Therefore, the Gi protein is located at nucleotide 1,066 through 2,133 (see, SEQ.ID.NO.:13) and at amino acid residue 356 through 711 (see, SEQ.ID.NO.:14). Those skilled in the art are credited with the ability to select techniques for constructing a GPCR Fusion Protein where the G protein is fused to the 3' end of the GPCR of interest.

Example 3583

ASSAY FOR DETERMINATION OF CONSTITUTIVE ACTIVITY OF NON-ENDOGENOUS GPCRS

A. Intracellular IP_3 Accumulation Assay

On day 1, cells comprising the receptors (endogenous and/or non-endogenous) can be plated onto 24 well plates, usually 1×10^5 cells/well (although this number can be optimized). On day 2 cells can be transfected by firstly mixing 0.25 μ g DNA in 50 μ l serum free DMEM/well and 2 μ l lipofectamine in 50 μ l serum-free DMEM/well. The solutions are gently mixed and incubated for 15-30 min at room temperature. Cells are washed with 0.5 ml PBS and 400 μ l of serum free media is mixed with the transfection media and added to the cells. The cells are then incubated for 3-4 hrs at $37^\circ\text{C}/5\%\text{CO}_2$ and then the transfection media is removed and replaced with 1ml/well of regular growth media. On day 3 the cells are labeled with ^3H -myo-inositol. Briefly, the media is removed and the cells are washed with 0.5 ml PBS. Then 0.5 ml inositol-free/serum free media (GIBCO BRL) is added/well with 0.25 μCi of ^3H -myo-inositol/ well and the cells are incubated for 16-18 hrs o/n at $37^\circ\text{C}/5\%\text{CO}_2$. On Day 4 the cells are washed with 0.5 ml PBS and 0.45 ml of assay medium is added containing inositol-free/serum free media 10 μM pargyline 10 mM lithium chloride or 0.4 ml of assay medium and 50 μ l of 10x

ketanserin (ket) to final concentration of 10 μ M. The cells are then incubated for 30 min at 37°C. The cells are then washed with 0.5 ml PBS and 200 μ l of fresh/ice cold stop solution (1M KOH; 18 mM Na-borate; 3.8 mM EDTA) is added/well. The solution is kept on ice for 5-10 min or until cells were lysed and then neutralized by 200 μ l of fresh/ice cold neutralization sol. (7.5 % HCL). The lysate is then transferred into 1.5 ml eppendorf tubes and 1 ml of chloroform/methanol (1:2) is added/tube. The solution is vortexed for 15 sec and the upper phase is applied to a Biorad AG1-X8™ anion exchange resin (100-200 mesh). Firstly, the resin is washed with water at 1:1.25 W/V and 0.9 ml of upper phase is loaded onto the column. The column is washed with 10 mls of 5 mM myo-inositol and 10 ml of 5 mM Na-borate/60mM Na-formate. The inositol tris phosphates are eluted into scintillation vials containing 10 ml of scintillation cocktail with 2 ml of 0.1 M formic acid/ 1 M ammonium formate. The columns are regenerated by washing with 10 ml of 0.1 M formic acid/3M ammonium formate and rinsed twice with H₂O and stored at 4°C in water.

Reference is made to Figure 1. Figure 1 provides an illustration of IP₃ production from several non-endogenous, constitutively activated version of MCH receptor as compared with the endogenous version of this receptor. When compared to the endogenous version of MCH receptor ("MCH-R wt"), MCH-IC3-SST2 evidenced about a 27% increase in IP₃ accumulation.

Example 3584

Determination of Compound Using [³⁵S]GTP γ S ASSAY

Direct identification of candidate compounds was initially screened using [³⁵S]GTP γ S Assay (see, Example 6 of co-pending patent application 09/826,509). Preferably, an MCH receptor: Gi Fusion Protein was utilized, according to Example 6(2) of co-pending patent application 09/826,509. Several lead hits were identified utilizing [³⁵S]GTP γ S Assay.

Example 3585

High Throughput Functional Screening: FLIPR™

Subsequently, a functional based assay was used to confirm the lead hits, referred to as FLIPR™ (the Fluorometric Imaging Plate Reader) and FDSS6000™ (Functional

Drug Screening System). This assay utilized a non-endogenous version of the MCH receptor, which was created by swapping the third intracellular loop of the MCH receptor with that of the SST2 receptor (see Example 2(B)(2) of patent application serial number 09/826,509).

The FLIPR and FDSS assays are able to detect intracellular Ca^{2+} concentration in cells, which can be utilized to assess receptor activation and determine whether a candidate compound is an, for example, antagonist, inverse agonist or agonist to a Gq-coupled receptor. The concentration of free Ca^{2+} in the cytosol of any cell is extremely low, whereas its concentration in the extracellular fluid and endoplasmic reticulum (ER) is very high. Thus, there is a large gradient tending to drive Ca^{2+} into the cytosol across both the plasma membrane and ER. The FLIPRTM and FDSS6000TM systems (Molecular Devices Corporation, HAMAMATSU Photonics K.K.) are designed to perform functional cell-based assays, such as the measurement of intracellular calcium for high-throughput screening. The measurement of fluorescent is associated with calcium release upon activation of the Gq-coupled receptors. Gi or Go coupled receptors are not as easily monitored through the FLIPRTM and FDSS6000TM systems because these G proteins do not couple with calcium signal pathways.

To confirm the lead hits identified using the [³⁵S]GTPγS assay, Fluorometric Imaging Plate Reader system was used to allow for rapid, kinetic measurements of intracellular fluorescence in 96 well microplates (or 384 well microplates). Simultaneous measurements of fluorescence in all wells can be made by FLIPR or FDSS6000TM every second with high sensitivity and precision. These systems are ideal for measuring cell-based functional assays such as monitoring the intracellular calcium fluxes that occur within seconds after activation of the Gq coupled receptor.

Briefly, the cells are seeded into 96 well at 5.5×10^4 cells/well with complete culture media (Dulbecco's Modified Eagle Medium with 10 % fetal bovine serum, 2 mM L-glutamine, 1 mM sodium pyruvate and 0.5 mg/ml G418, pH 7.4) for the assay next day. On the day of assay, the media is removed and the cells are incubated with 100 μl of loading buffer (4 μM Fluo4-AM in complete culture media containing 2.5 mM Probenicid, 0.5 mg/ml and 0.2% bovine serum albumin) in 5% CO₂ incubator at 37°C for 1 hr. The loading buffer is removed, and the cells are washed with wash buffer (Hank's Balanced Salt Solution containing 2.5 mM Probenicid, 20 mM HEPES, 0.5 mg/ml and 0.2% bovine

serum albumin, pH 7.4)). One hundred fifty μ l of wash buffer containing various concentrations of test compound are added to the cells, and the cells are incubated in 5% CO₂ incubator at 37°C for 30 min. Fifty μ l of wash buffer containing various concentration of MCH are added to each well, and transient changes in [Ca²⁺]_i evoked by MCH are monitored using the FLIPR or FDSS in 96 well plates at Ex. 488 nm and Em. 530 nm for 290 second. When antagonist activity of compound is tested, 50 nM of MCH is used.

Use of FLIPRTM and FDSS6000TM can be accomplished by following manufacturer's instruction (Molecular Device Corporation and HAMAMATSU Photonics K.K.).

The results were shpwn below.

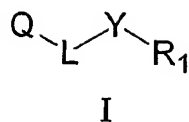
Compound No.	IC ₅₀ value (nM)
Example 41	6
Example 42	19

It is intended that each of the patents, applications, printed publications, and other published documents mentioned or referred to in this specification be herein incorporated by reference in their entirety.

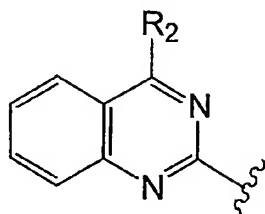
Those skilled in the art will appreciate that numerous changes and modifications may be made to the preferred embodiments of the invention and that such changes and modifications may be made without departing from the spirit of the invention. It is therefore intended that the appended claims cover all such equivalent variations as fall within the true spirit and scope of the invention.

What is claimed is:

1. A compound of Formula I:

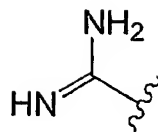


wherein Q is



II

or



III

R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

•halogen,

•hydroxy,

•oxo,

•C₁-C₃ alkoxy,

•C₁-C₃ alkoxy substituted by substituent(s) independently selected from

••carbocyclic aryl,

••heterocyclyl,

••heterocyclyl substituted by C₁-C₃ alkyl,

•C₁-C₃ alkylcarbonyloxy,

•carbocyclyloxy,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

••carbocyclic aryl,

••carbocyclic aryl substituted by C₁-C₃ alkoxy,

- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
- oxo,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
- carbocyclic arylcarbonylamino,
- halogenated carbocyclic arylcarbonylamino,
- heterocycloxy,
- heterocycloxy substituted by C₁-C₃ alkyl,
- substituted heterocyclyl-ethylideneaminooxy,
- C₁-C₃ alkoxy carbonyl,
- C₁-C₃ alkoxy carbonyl substituted by carbocyclic aryl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
- cyano,
- carbocyclic aryl,
- heterocyclyl,
- mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
- hydroxy,
- C₁-C₃ alkyl,
- C₁-C₃ alkylcarbonylamino,
- C₁-C₃ alkylcarbonylamino substituted by substituent(s) independently selected from
- C₁-C₃ alkylcarbonylamino,
- carbocyclic arylcarbonylamino,
- heterocyclyl,
- C₁-C₄ alkoxy carbonylamino,
- heterocyclyl carbonylamino,
- carbocyclic arylsulfonylamino,

- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
- carbocyclic arylsulfonyl,
- halogenated carbocyclic arylsulfonyl,
- heterocyclylthio,
- heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
 - C₃-C₆ cycloalkenyl,
 - carbocyclyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₂-C₃ alkenyl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-carbocyclic arylamino,

- halogenated mono- or di-carbocyclic arylamino,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - mercapto,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- hydroxy,
- nitro,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- heterocyclyl,

•heterocyclyl substituted by substituent(s) independently selected from

- hydroxy,
- nitro,
- C₁-C₃ alkyl,
- C₁-C₃ alkoxy,

(iii) C₂-C₄ alkynyl,

C₂-C₄ alkynyl substituted by carbocyclic aryl,

(iv) C₃-C₆ cycloalkyl,

C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from

- C₁-C₃ alkyl,
- C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
- mono- or di-C₁-C₃ alkylamino,
- mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
- carbocyclic arylcarbonylamino,
- carbocyclic aryl,

(v) C₃-C₆ cycloalkyl,

C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,

(vi) carbocyclyl,

carbocyclyl substituted by substituent(s) independently selected from

- hydroxy,

- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,

- C₂-C₃ alkenyl substituted by carbocyclic aryl,
- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- C₂-C₃ alkenyloxy,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - halogenated C₁-C₄ alkyl,
 - C₁-C₃ alkoxy,
 - heterocyclyloxy,
 - heterocyclyloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,

- carboxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- mono- or di-carbocyclic arylaminocarbonyl,
- mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkynylcarbonylamino,
- C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- carbocyclic aryl diazo,
- carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - cyano,
 - C₁-C₃ alkyl,
 - heterocyclylthio,
 - C₁-C₃ alkylsulfonyl,
 - mono- or di-C₁-C₃ alkylaminosulfonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocyclic arylcarbonylamino,
 - halogenated carbocyclic arylcarbonylamino,
 - C₁-C₃ alkoxycarbonyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₄ alkylcarbonylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - halogenated carbocyclic arylthio,
 - carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - C₁-C₃ alkoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - halogen,

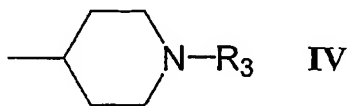
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl;

R₂ is -NHNH₂, -NHNHBoc, -N(R_{2a})(R_{2b}), morpholino, 4-acetyl-piperazyl, or 4-phenyl-piperazyl;

wherein R_{2a} is H or C₁-C₃ alkyl;

R_{2b} is C₁-C₄ alkyl, C₁-C₄ alkyl substituted by substituent(s) independently selected from

- hydroxy,
 - C₁-C₃ alkoxy,
 - amino,
 - NHBoc,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - SO₂NH₂,
 - heterocyclyl,
- C₃-C₆ cycloalkyl, carbocyclic aryl, carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- or a group of Formula IV;

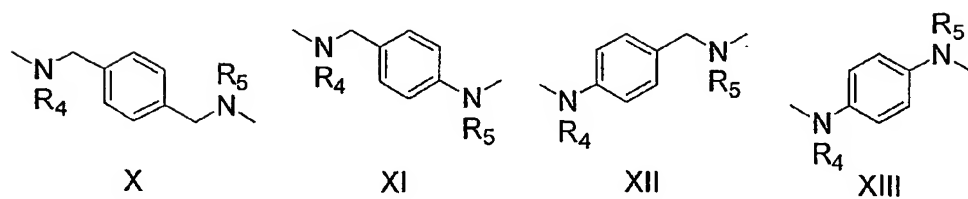
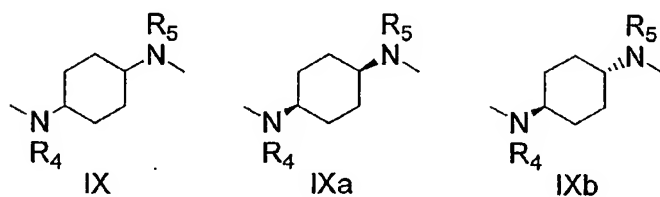
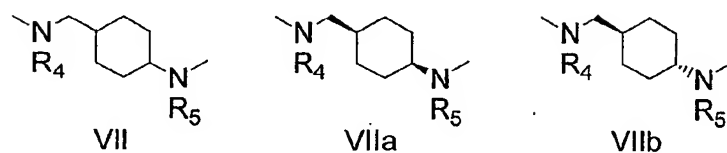
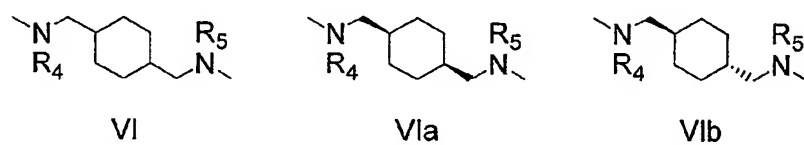
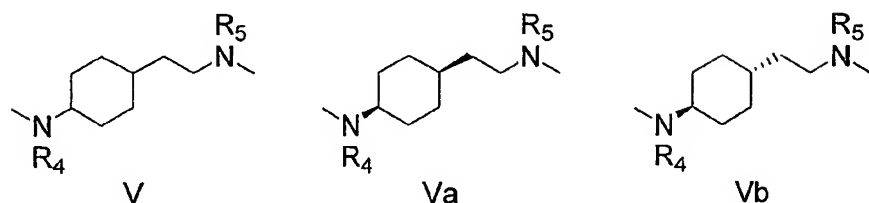


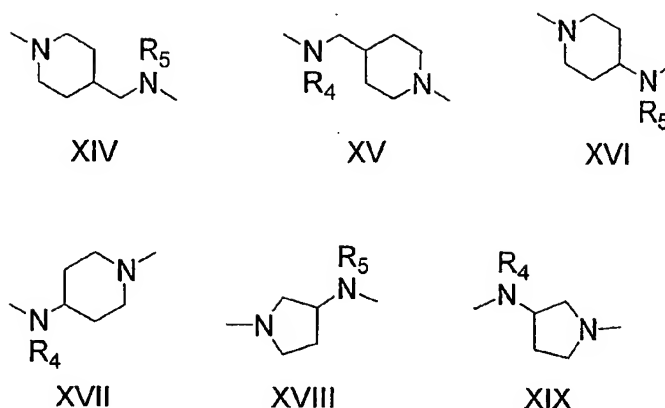
wherein Boc is carbamic acid *tert*-butyl ester and R₃ is C₁-C₃ alkyl or C₁-C₃ alkyl

substituted by substituent(s) independently selected from

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by C₁-C₃ alkoxy;

L is selected from Formula V - XIX;





wherein R_4 is H or C_1 - C_3 alkyl;

R_5 is H, C_1 - C_3 alkyl, or C_1 - C_3 alkyl substituted by a substituted carbocyclic aryl;

Y is $-S(O)_2-$, $-C(O)-$, or $-(CH_2)_m$;

m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, biphenyl, or phenanthryl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl, 9H-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, C-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isoindolyl, 1,3-dioxolanyl, 1H-indolyl, 1H-pyrrolo[2,3-c]pyridyl, 1H-pyrrolyl, 1-oxo-3H-isobenzofuranyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2H-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2H-benzo[1,4]oxazinyl, 3,4-dihydro-2H-benzo[b][1,4]dioxepinyl, 4H-benzo[1,3]dioxinyl, 4H-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9H-carbazolyl, 9H-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, benzofuryl, benzothiazolyl, cinnolyl, furyl, imidazo[2,1-b]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperazyl, piperidyl, piridyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-

dihydro-benzofuryl, tetrahydro-thienyl, or benzofuranyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

2. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

•halogen,

•oxo,

•C₁-C₃ alkoxy,

•C₁-C₃ alkoxy substituted by carbocyclic aryl,

•C₁-C₃ alkylcarbonyloxy,

•carbocyclyloxy,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C₁-C₄ alkyl,

••C₁-C₄ alkyl substituted by substituent(s) independently selected from

•••oxo,

•••carbocyclic arylcarbonylamino,

•••halogenated carbocyclic arylcarbonylamino,

•heterocyclyloxy,

•heterocyclyloxy substituted by C₁-C₃ alkyl,

•substituted heterocyclyl-ethylideneaminooxy,

•C₁-C₃ alkoxycarbonyl,

•C₁-C₃ alkoxycarbonyl substituted by carbocyclic aryl,

•mono- or di-C₁-C₃ alkylaminocarbonyl,

•mono- or di-carbocyclic arylamino,

•mono- or di-carbocyclic arylamino substituted by hydroxy,

•C₁-C₃ alkylcarbonylamino,

- C₁-C₃ alkylcarbonylamino substituted by substituent(s) independently selected from
 - C₁-C₃ alkylcarbonylamino,
 - carbocyclic arylcarbonylamino,
 - heterocyclyl,
- C₁-C₄ alkoxy carbonylamino,
- heterocyclyl carbonylamino,
- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylaminocarbonyl,
 - halogenated mono- or di-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - heterocyclylthio,
 - heterocyclylthio substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
- C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
- C₃-C₆ cycloalkenyl,

- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkylcarbonyloxy,
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,

- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- mercapto,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- C₁-C₃ alkylsulfonyl,
- C₃-C₆ cycloalkyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₆ alkenyl,
C₂-C₆ alkenyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - hydroxy,

- C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- (iii) C₃-C₆ cycloalkyl,
C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - carbocyclic arylcarbonylamino,
 - carbocyclic aryl,
 - (iv) carbocyclyl,
carbocyclyl substituted by nitro,
 - (v) carbocyclic aryl,
carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryloxy,
 - carbocyclylimino,
 - carbocyclylimino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl,

- heterocyclyl,
- heterocyclyl substituted by C₁-C₃ alkyl,
- C₁-C₇ alkoxy,
- C₁-C₇ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - C₁-C₃ alkylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by C₁-C₃ alkoxy,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₃ alkylaminocarbonyl,
 - mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylaminocarbonyl,
 - mono- or di-carbocyclic arylaminocarbonyl substituted by C₁-C₃ alkyl,
 - amino,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkynylcarbonylamino,
 - C₁-C₃ alkynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino,
 - carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
 - (carbocyclic aryl)NHC(O)NH,
 - (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by cyano,
 - C₁-C₃ alkylsulfonyl,
 - mono- or di-C₁-C₃ alkylaminosulfonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,

- halogenated C₁-C₇ alkyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (vi) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by carbocyclic aryl,
 - C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - halogenated carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,

- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -C(O)-;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 10,11-dihydro-5-oxo-dibenzo[a,d]cycloheptyl, 1-oxo-indanyl, 9*H*-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, *C*-fluoren-9-ylidene, indanyl, indenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isindolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, cinnoyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxazolyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

3. A compound according to claim 2, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
 - C₅-C₆ cycloalkyl,
 - C₅-C₆ cycloalkenyl,
 - carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from

- oxo,
- carbocyclic aryl,
- heterocyclyl,
- C₁-C₄ alkoxy,
- halogenated C₁-C₄ alkoxy,
- C₁-C₄ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated mono-carbocyclic arylaminocarbonyl,
- carbocyclic aryl,
- heterocyclyl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl,
 - C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,

- cyano,
- nitro,
- C₁-C₉ alkyl,
- C₁-C₉ alkyl substituted by substituent(s) independently selected from
- halogen,
- oxo,
- carbocyclic aryl,
- carbocyclic aryl substituted by methyl,
- carbocyclic aryloxy,
- C₁-C₇ alkoxy,
- halogenated C₁-C₇ alkoxy,
- C₁-C₇ alkoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by methoxy,
- amino,
- di-methylamino,
- propargynylcarbonylamino substituted by carbocyclic aryl,
- carbocyclic arylsulfonylamino substituted by methyl,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
- halogenated methylthio,
- carbocyclic arylthio substituted by cyano,
- di-propylamino sulfonyl,
- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- C₁-C₄ alkyl,

- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein R₄ and R₅ are independently selected from H or C₁-C₃ alkyl;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxo-isoindolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 4-oxo-benzopyranyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl,

quinoxalyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isindolyl, 2,3-dihydro-benzofuryl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, cinnolyl, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

4. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
 - carbocyclic arylthio,
 - heterocyclylthio substituted by nitro,
 - heterocyclylthio substituted by methyl,
- C₅-C₆ cycloalkenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,

- ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₄ alkoxy,
 - halogenated C₁-C₄ alkoxy,
 - C₁-C₄ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,

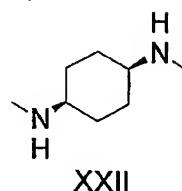
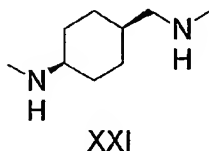
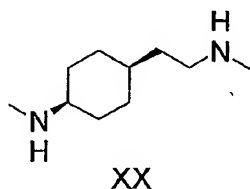
(iv) carbocyclyl,

(v) carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- hydroxy,
- cyano,
- nitro,
- C₁-C₉ alkyl,
- C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₇ alkoxy,
 - halogenated C₁-C₇ alkoxy,
 - C₁-C₇ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,
 - mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - heterocyclyl substituted by methyl,
 - heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from

- halogen,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - methylthio substituted by halogenated carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - methoxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methyl,
 - C₁-C₃ alkylthio,
 - propenylthio,
 - carbocyclic arylthio,
 - C₁-C₃ alkylsulfonyl,
 - carbocyclic arylsulfonyl,
 - carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryl substituted by nitro,
 - heterocyclyl;

L is selected from Formula XX - XXII;



wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, 9-oxo-fluorenyl, indenyl, anthraquinonyl, C-fluoren-

9-ylidene, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 4-oxo-benzopyranyl, azetidiny, benzo[b]thienyl, furyl, isoxazolyl, morpholinyl, piperidyl, piridyl, pyrazolyl, pyridyl, quinolyl, thiazolidyl, thiazolyl, thienyl, thiolanyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2-oxo-benzopyranyl, 2-oxo-pyrrolidinyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 9*H*-xanthenyl, cinnolyl, imidazolyl, morpholino, pyrimidyl, pyrrolidyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

5. A compound according to claim 4, wherein

R₁ represents

(i) C₁-C₅ alkyl substituted by substituent(s) independently selected from

- oxo,
- di-propylaminocarbonyl,
- methoxy substituted by carbocyclic aryl,
- methylcarbonyloxy,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- carbocyclic aryloxy substituted by nitro,
- heterocyclyloxy substituted by methyl,
- substituted heterocyclyl-ethylideneaminoxy,
- tert*-butoxycarbonylamino,
- carbocyclic arylcarbonylamino,
- C₁-C₂ alkylthio,
- C₁-C₂ alkylthio substituted by substituent(s) independently selected from
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methoxy,
- carbocyclic arylthio,
- heterocyclylthio substituted by nitro,
- heterocyclylthio substituted by methyl,

- cyclohexenyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - methyl,
 - methoxy,
 - ethenyl substituted by carbocyclic aryl substituted methylsulfinyl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - oxo,
 - carbocyclic aryl,
 - heterocyclyl,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryloxy,
 - halogenated mono-carbocyclic arylaminocarbonyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₂ alkyl,
 - C₁-C₂ substituted by carbocyclic aryl,
 - methoxy,
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (ii) C₂-C₃ alkenyl substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,

- carbocyclic aryl substituted by nitro,
- (iii) C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - methyl substituted by oxo,
 - methyl substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (iv) carbocyclyl,
- (v) carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₂ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - oxo,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methyl,
 - carbocyclic aryloxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - C₁-C₂ alkoxy substituted by carbocyclic aryl,
 - methylcarbonyloxy,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by methoxy,
 - amino,
 - di-methylamino,
 - propargynylcarbonylamino substituted by carbocyclic aryl,
 - carbocyclic arylsulfonylamino substituted by methyl,
 - (carbocyclic aryl)NHC(O)NH substituted by halogenated methoxy,
 - halogenated methylthio,
 - carbocyclic arylthio substituted by cyano,
 - di-propylamino sulfonyl,

- mono- or di- ethylaminocarbonyl substituted by carbocyclic aryl,
- carbocyclic aryl,
- heterocyclyl substituted by methyl,
- heterocyclyl substituted by halogenated carbocyclic aryl,
- (vi) or heterocyclyl substituted by substituent(s) independently selected from

- halogen,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
- halogen,
- methylthio substituted by halogenated carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- methoxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by methyl,
- C₁-C₃ alkylthio,
- propenylthio,
- carbocyclic arylthio,
- C₁-C₃ alkylsulfonyl,
- carbocyclic arylsulfonyl,
- carbocyclic arylsulfonyl substituted by methyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- carbocyclic aryl substituted by methyl,
- carbocyclic aryl substituted by nitro,
- heterocyclyl;

wherein carbocyclic aryl is phenyl, naphthyl, or biphenyl;

carbocyclyl is 1-oxo-indanyl, indenyl, 9-oxo-fluorenyl, 1,2,3,4-tetrahydro-naphthyl, or bicyclo[2.2.1]hepteny;

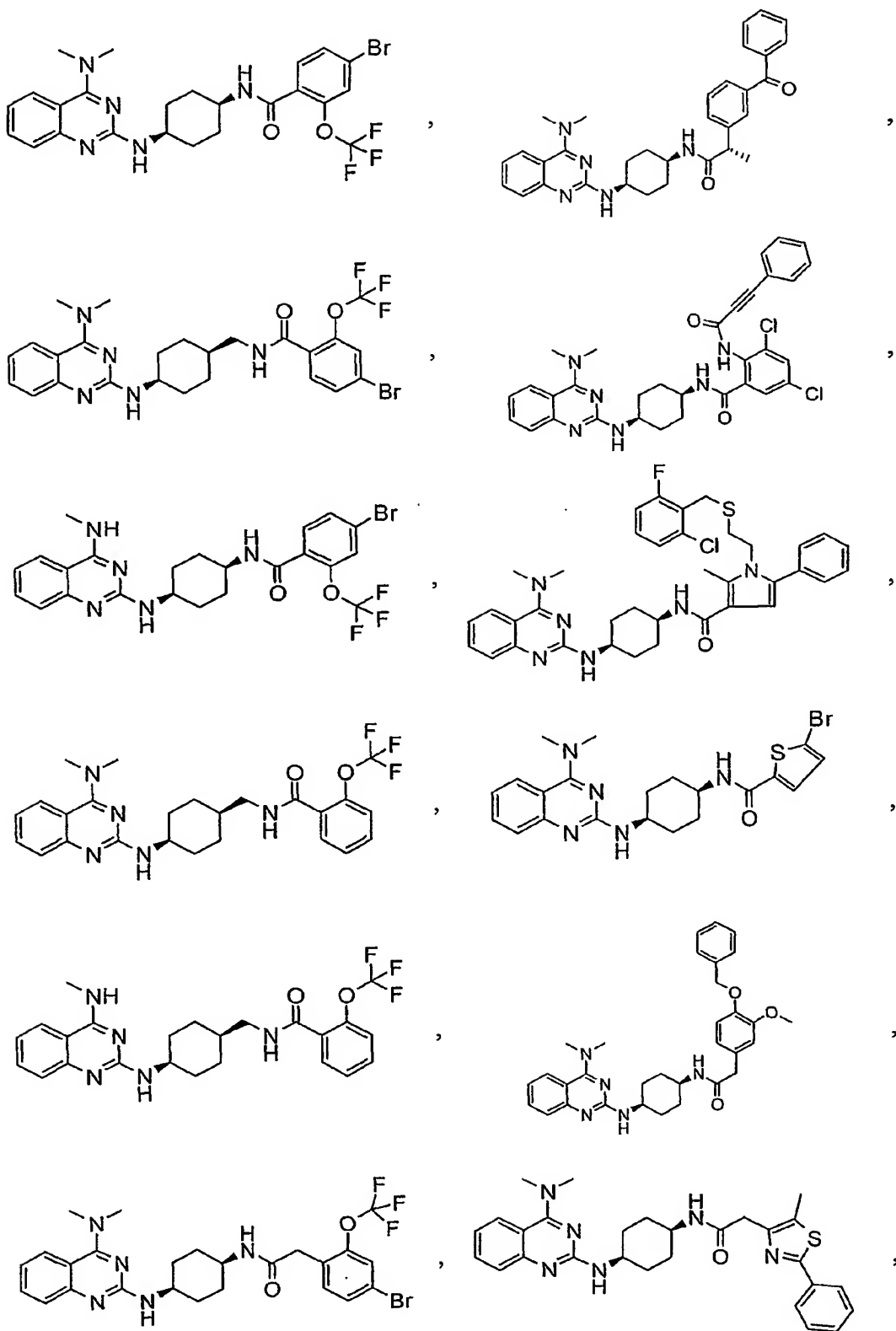
heterocyclyl is 1*H*-indolyl, 2,4-dihydro-3-oxo-pyrazolyl, furyl, pyrazolyl, pyridyl,

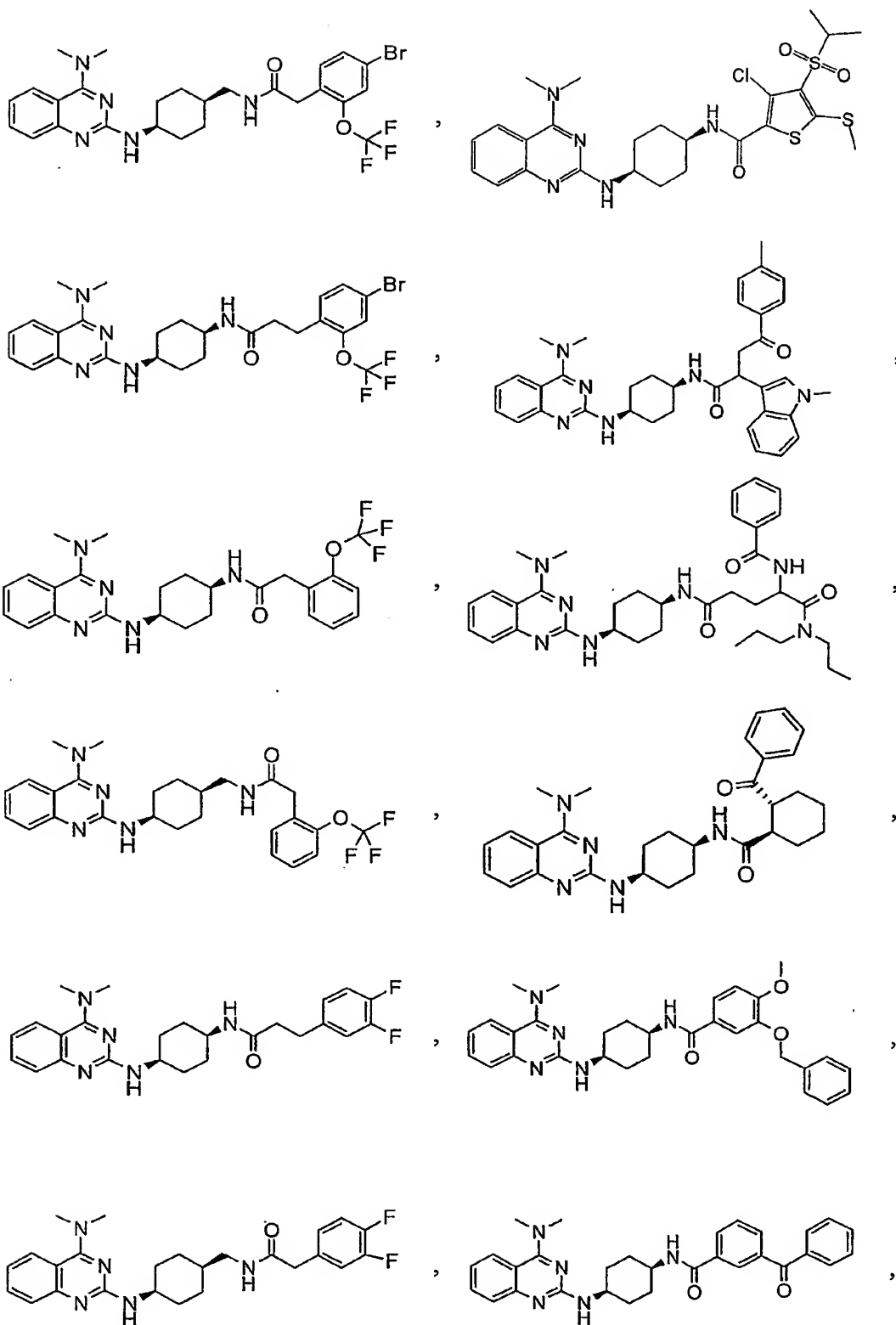
thienyl, 1,2,3-triazolyl, 1*H*-pyrrolyl, 2,3-dihydro-1-oxo-isoindolyl, 2,3-dihydro-benzofuryl, 2*H*-benzopyranyl, 2-oxo-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, pyrazolyl, pyrimidyl, quinolyl, thiazolyl, tetrahydro-thienyl, benzofuranyl, or benzothiazolyl;

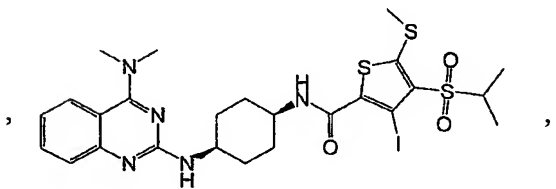
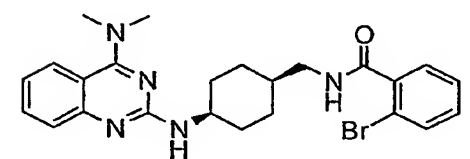
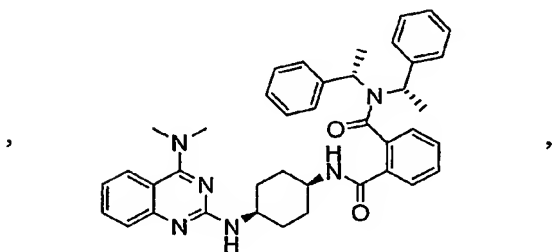
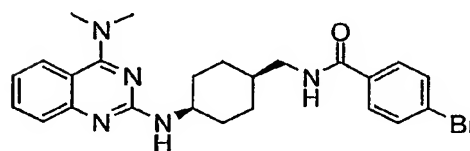
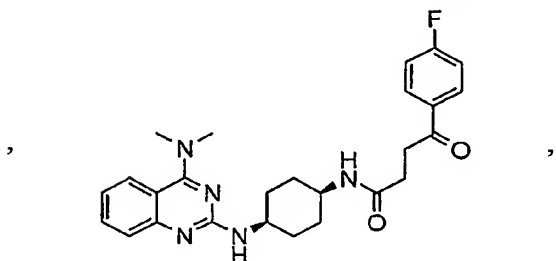
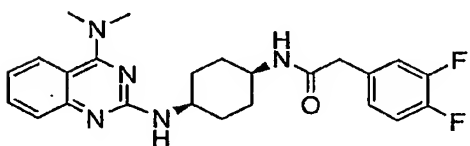
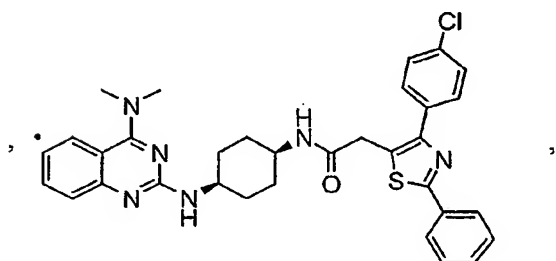
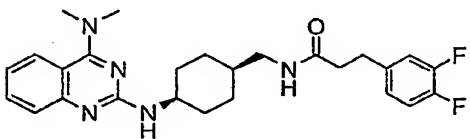
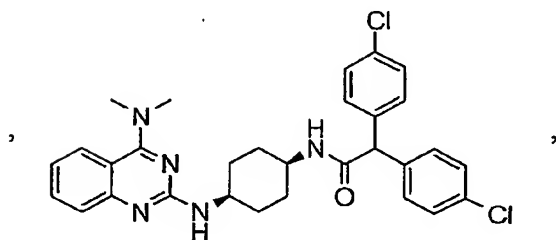
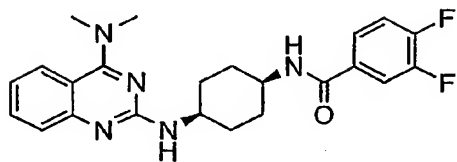
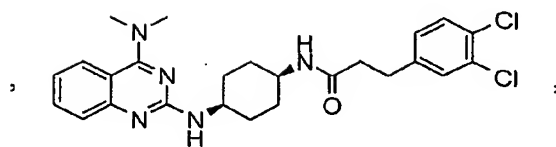
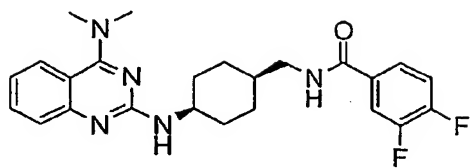
halogen is fluoro, chloro, bromo, or iodo;

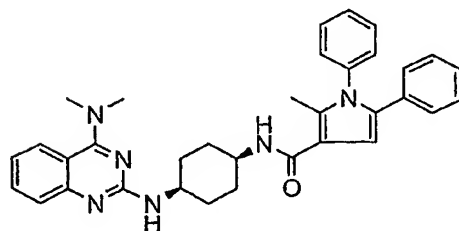
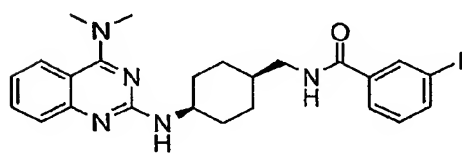
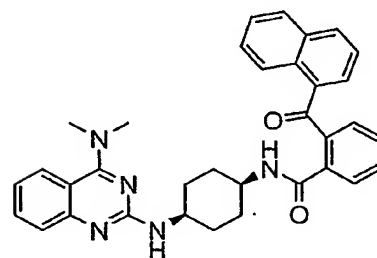
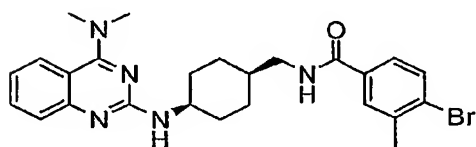
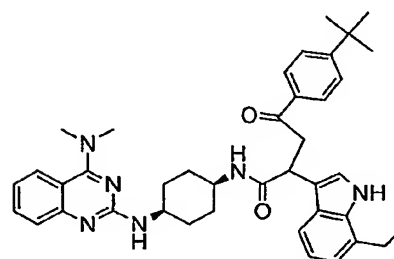
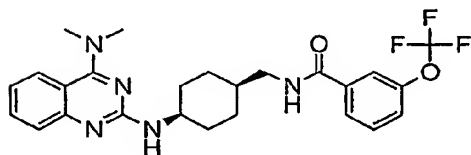
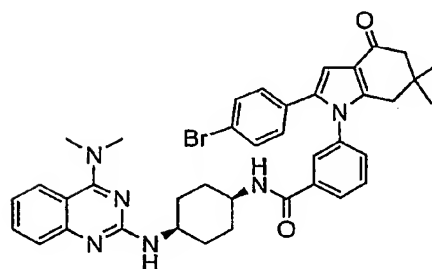
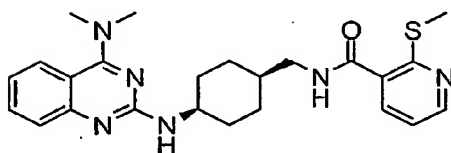
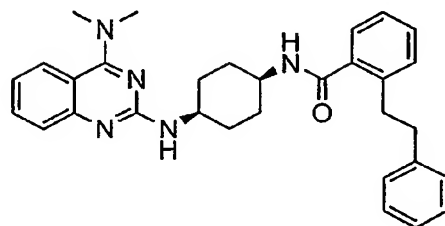
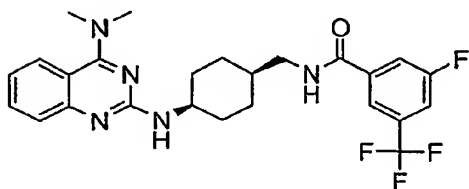
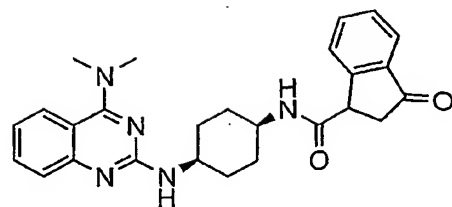
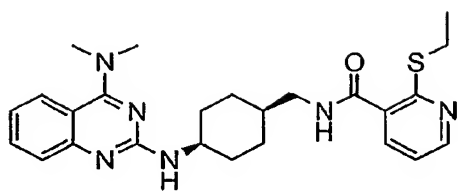
or a salt thereof.

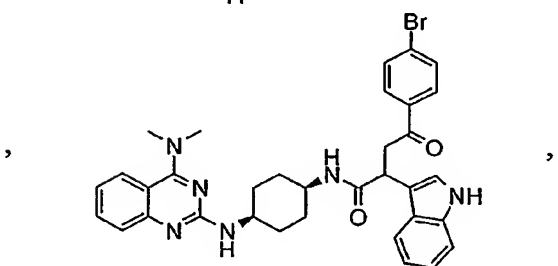
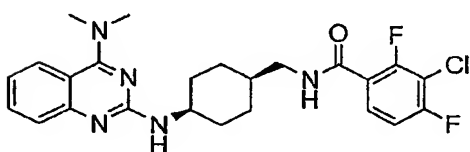
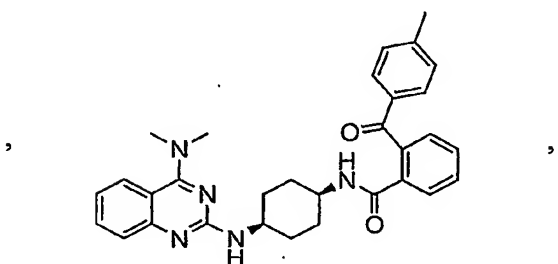
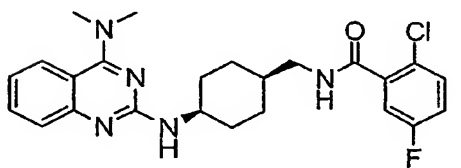
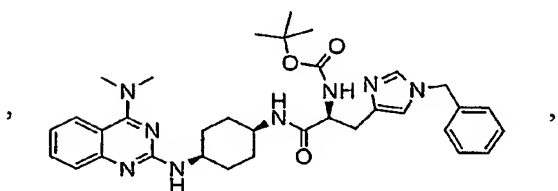
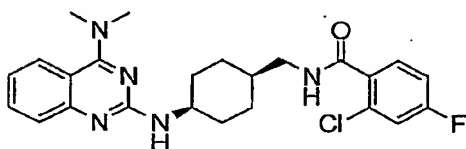
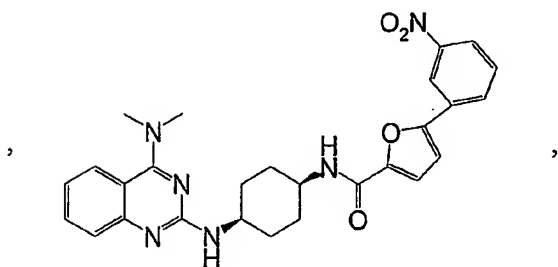
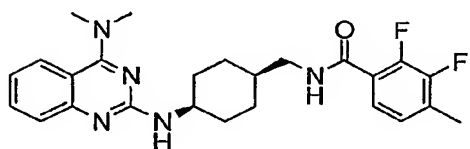
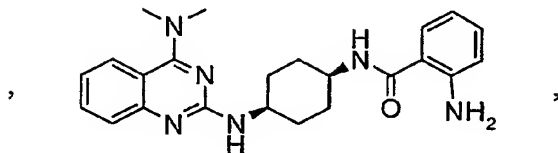
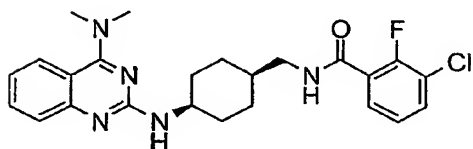
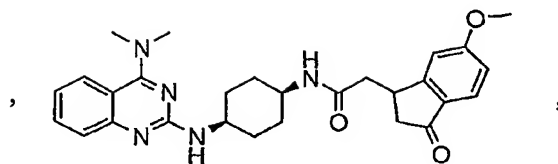
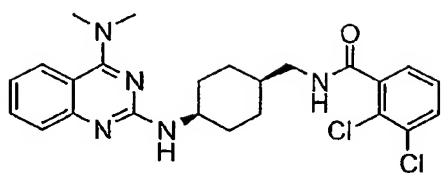
6. A compound according to claim 5 of Formula I selected from the group consisting of

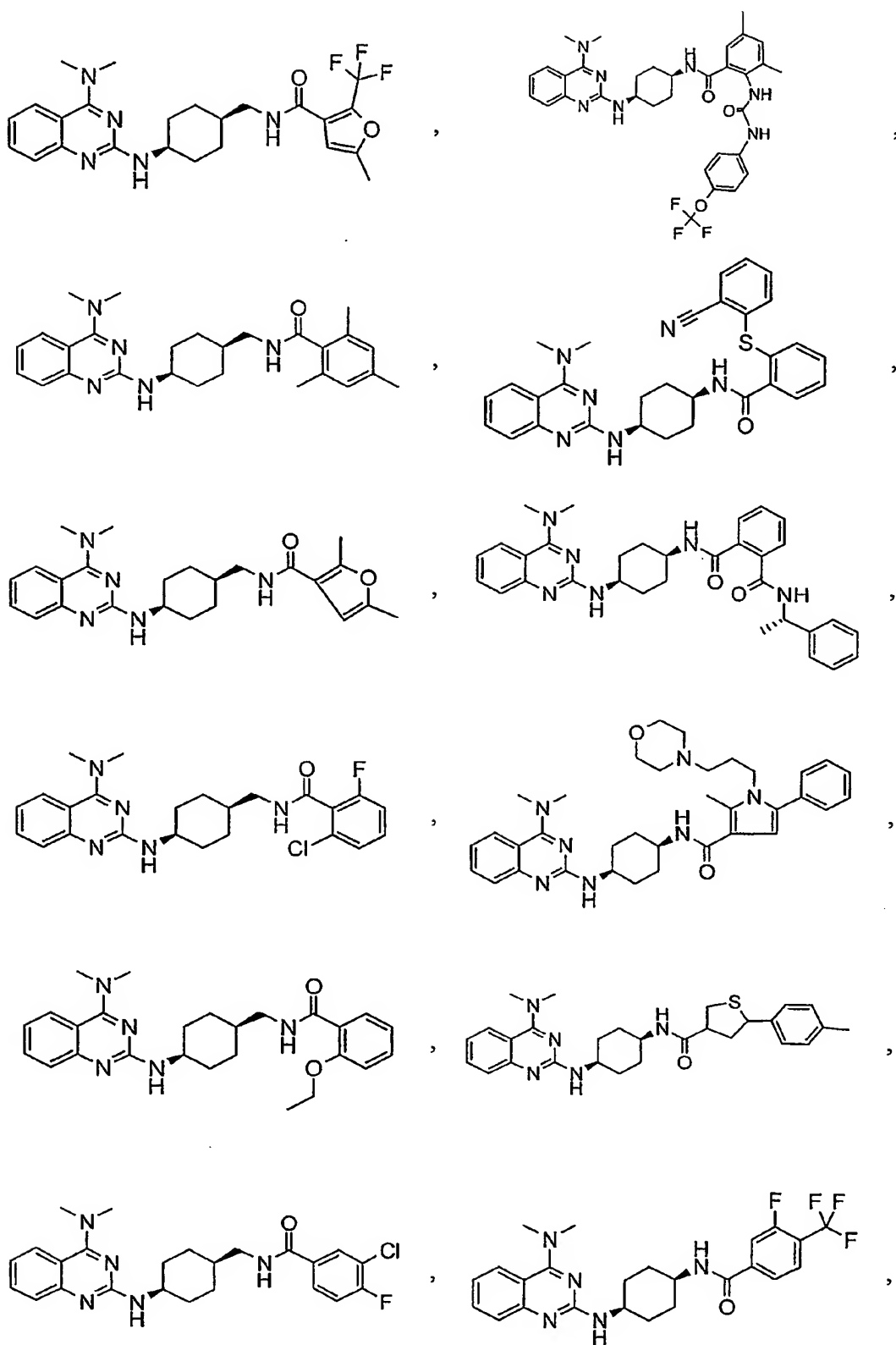


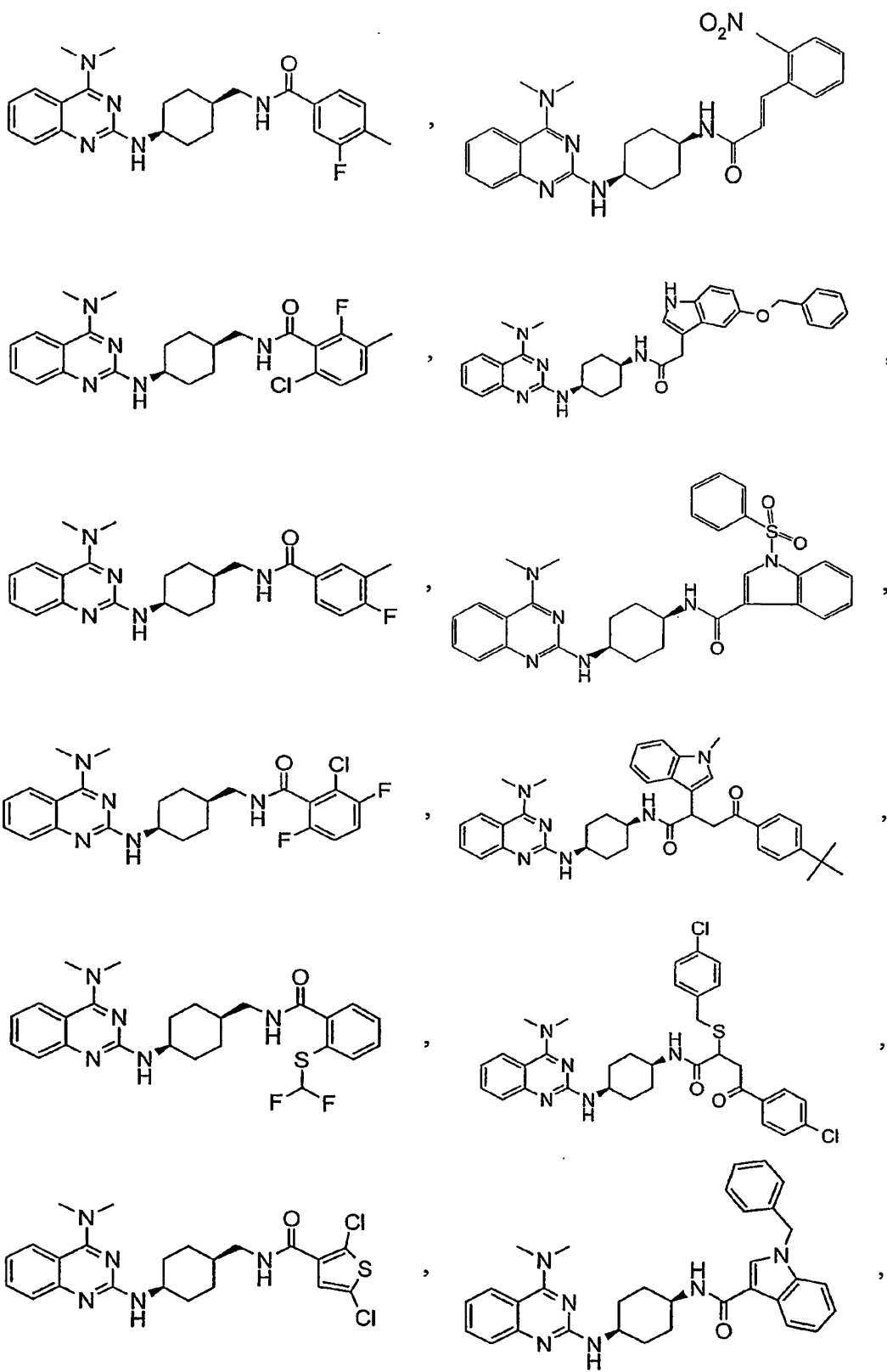


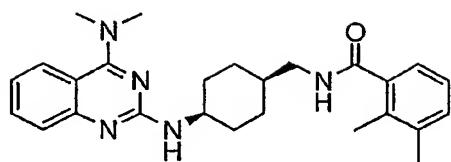




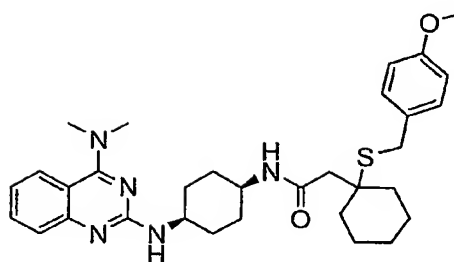




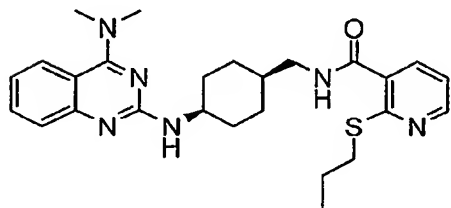




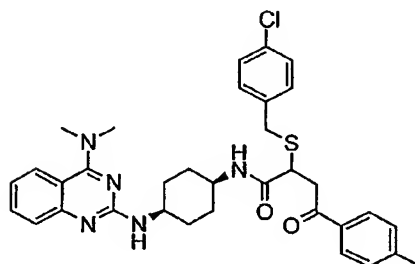
,



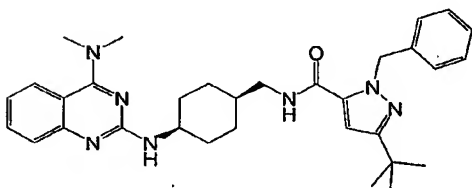
,



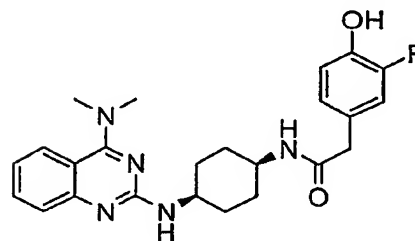
,



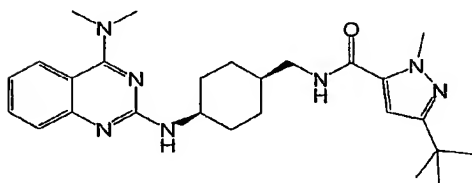
,



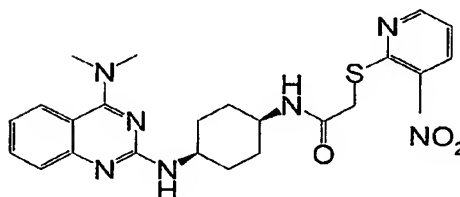
,



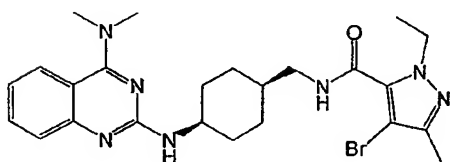
,



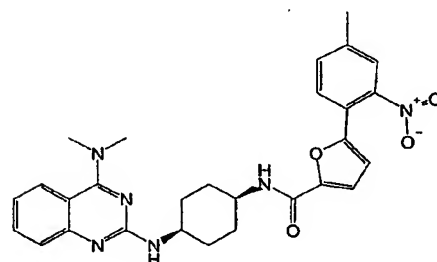
,



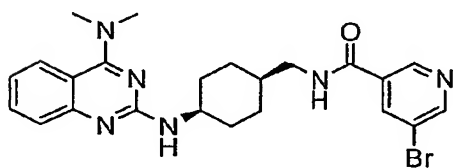
,



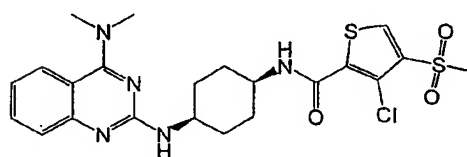
,



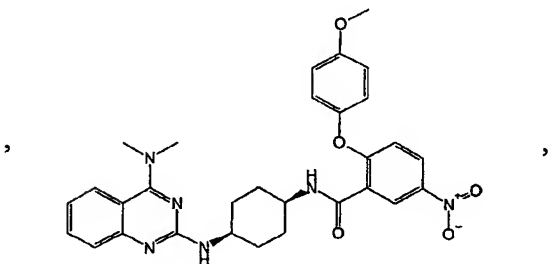
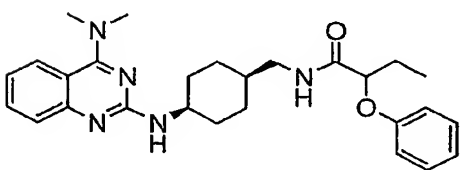
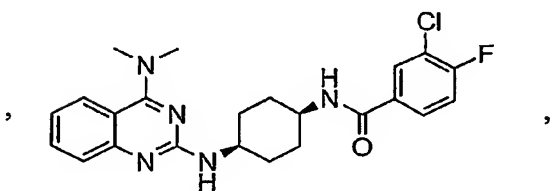
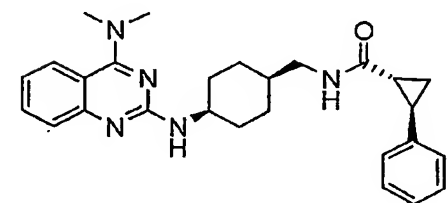
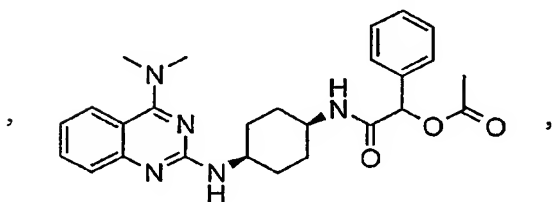
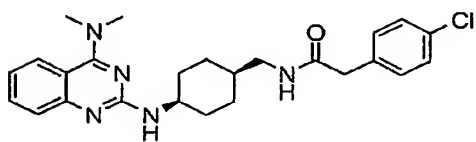
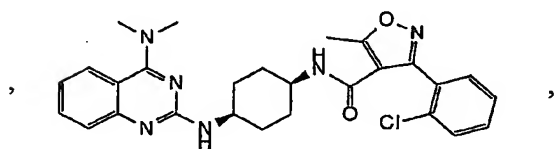
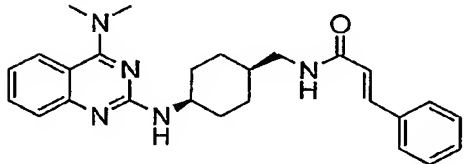
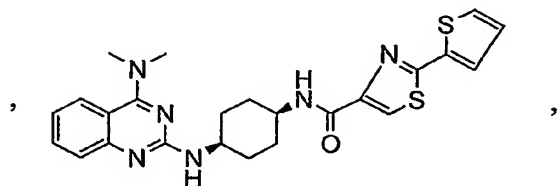
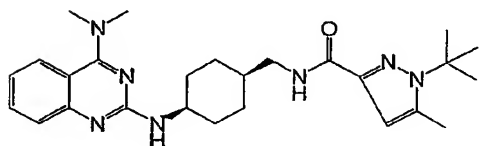
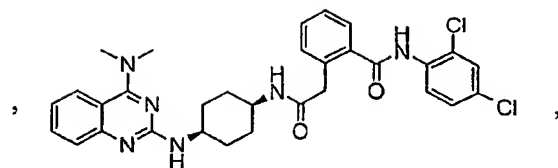
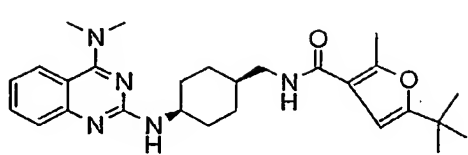
,

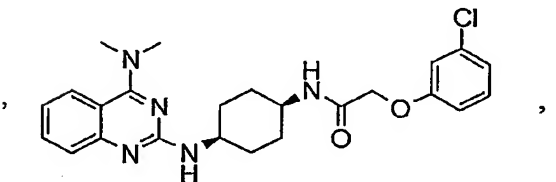
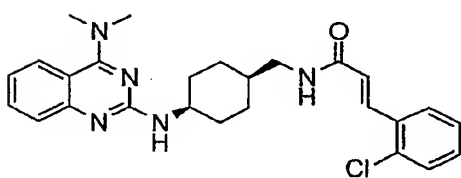
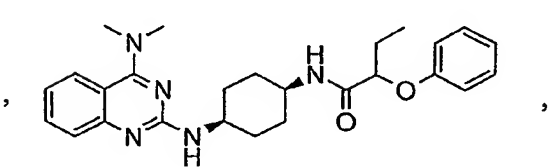
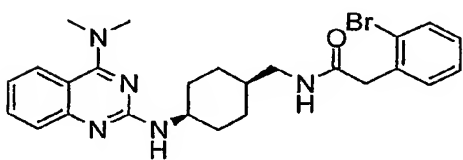
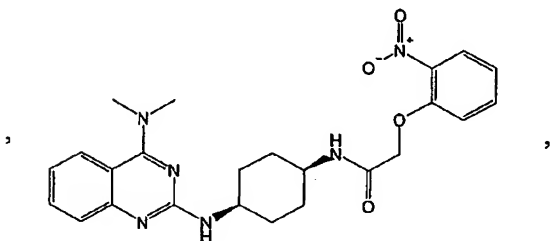
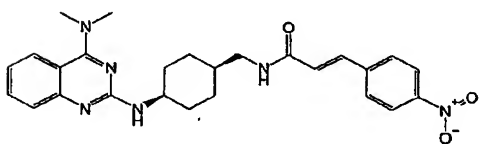
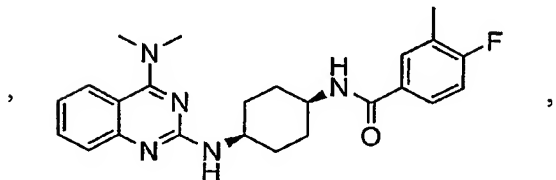
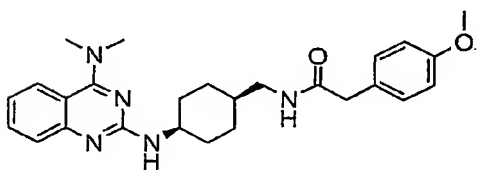
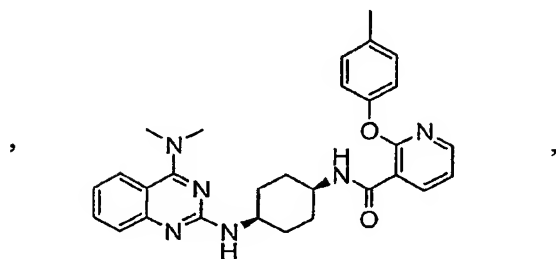
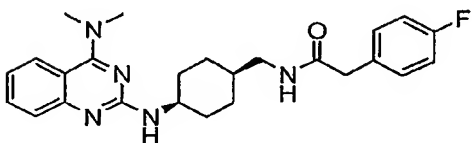
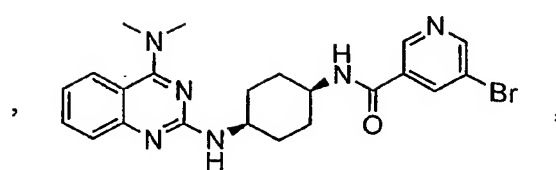
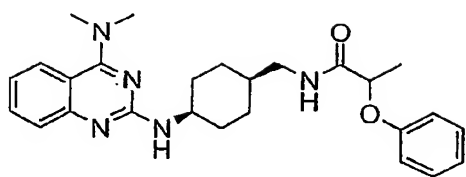


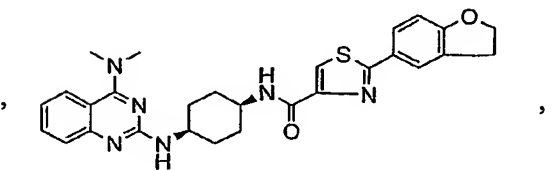
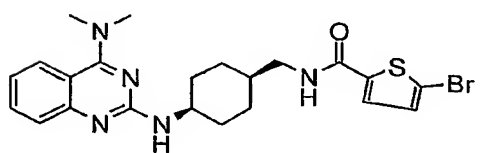
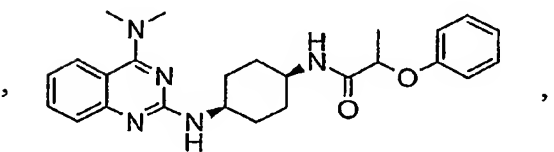
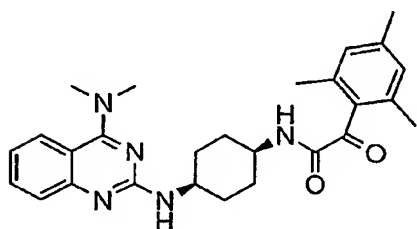
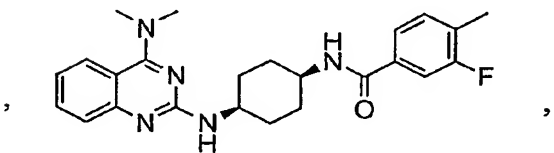
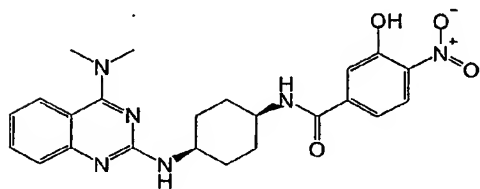
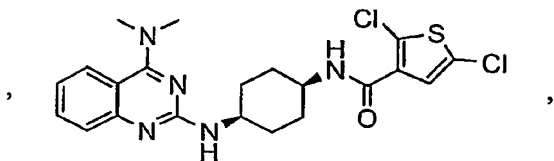
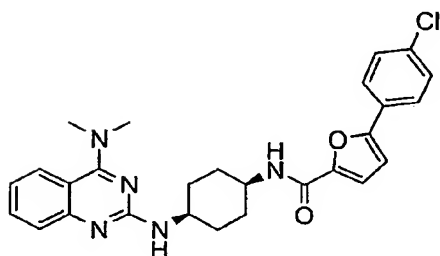
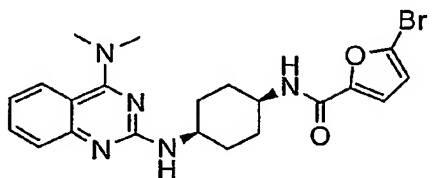
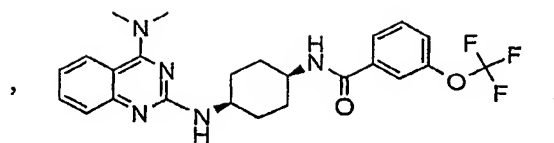
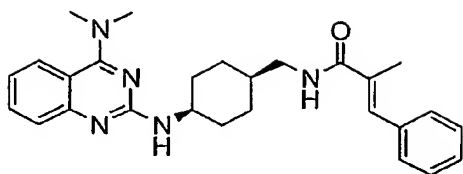
,

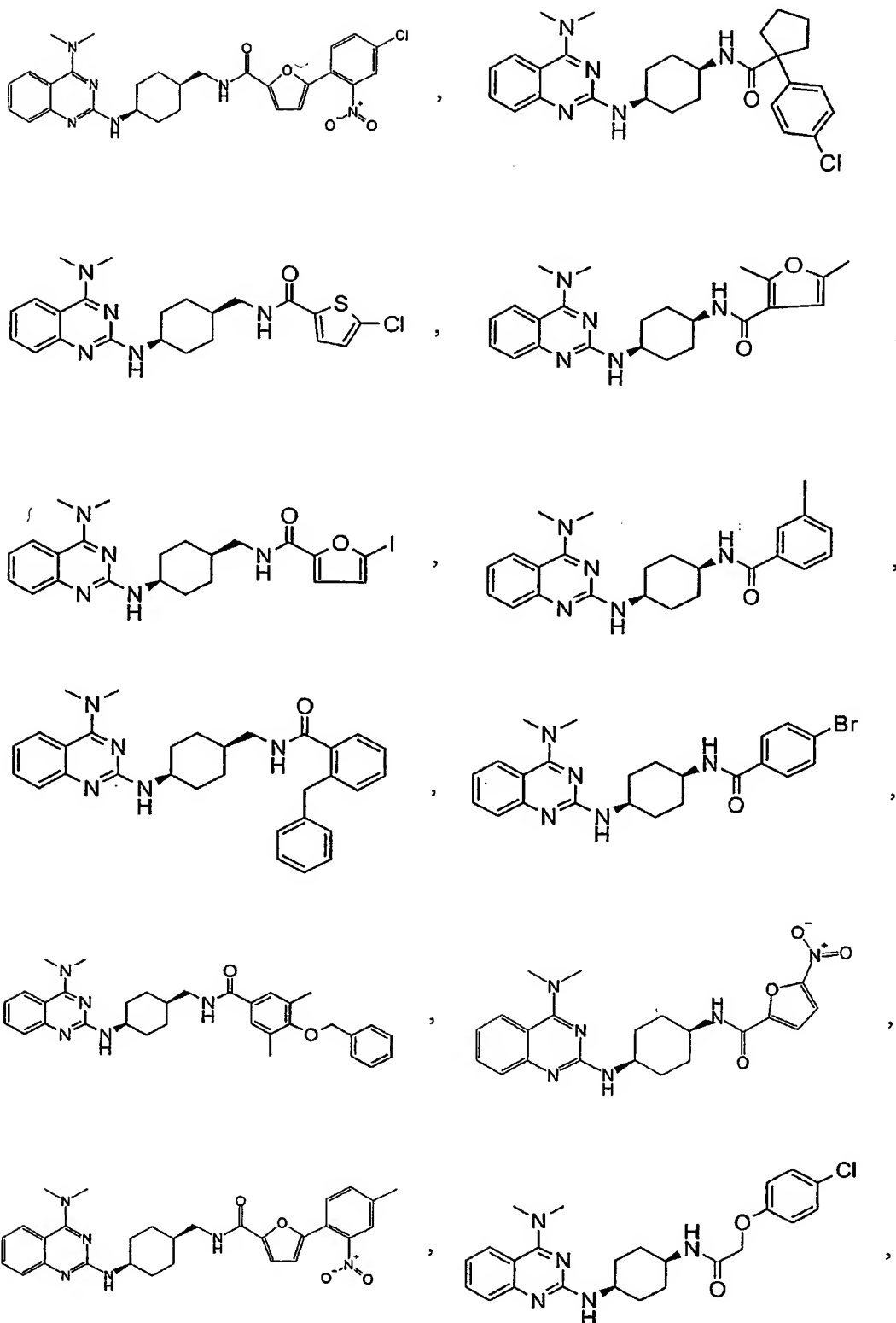


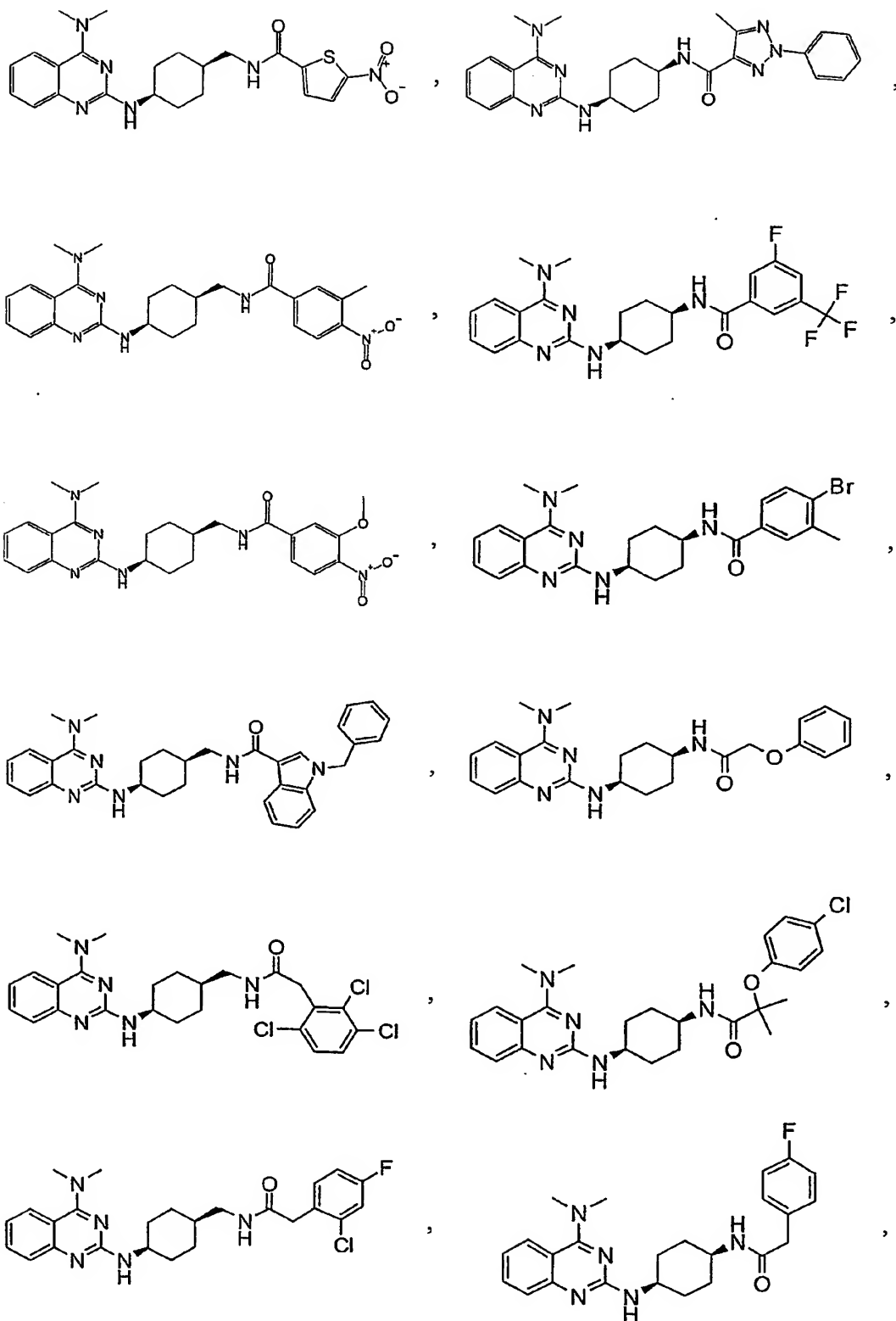
,

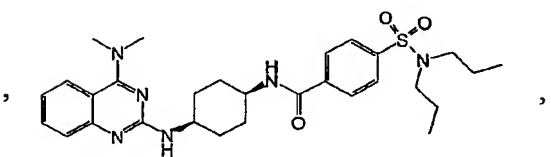
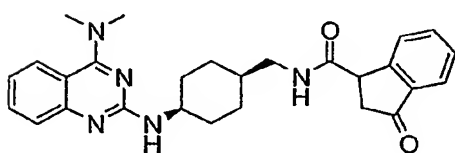
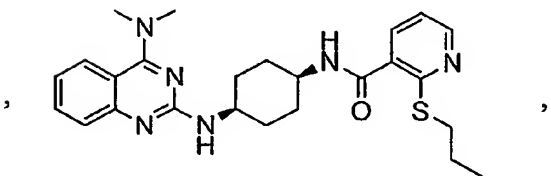
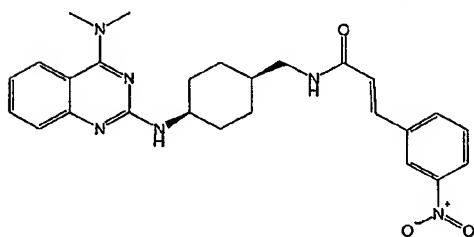
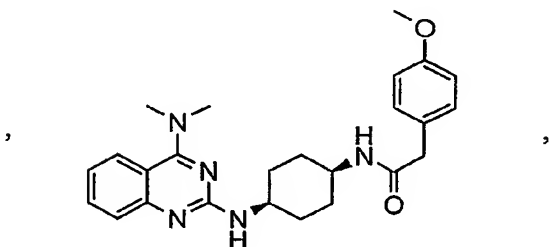
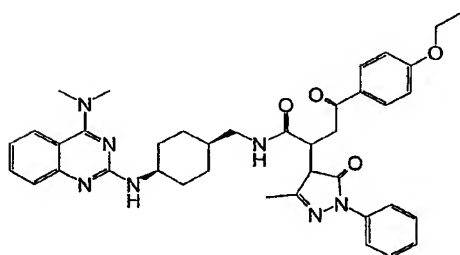
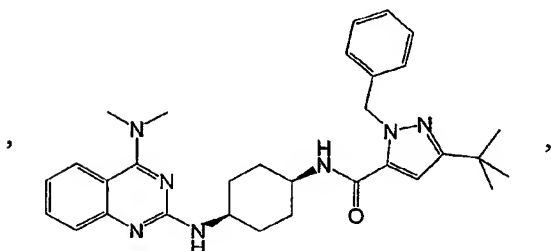
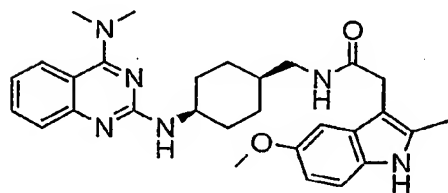
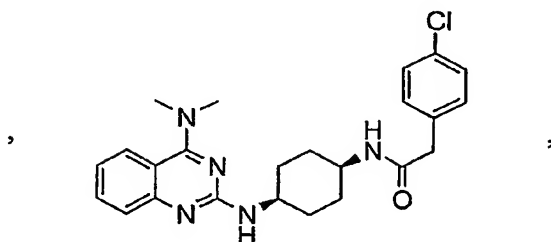
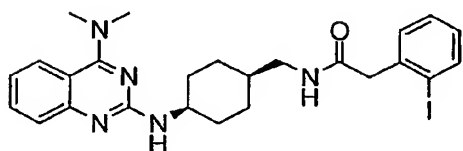
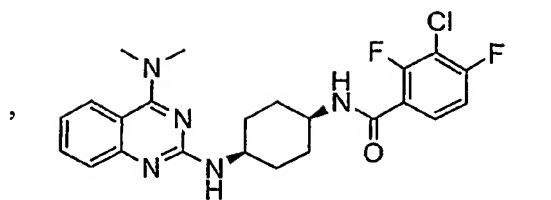
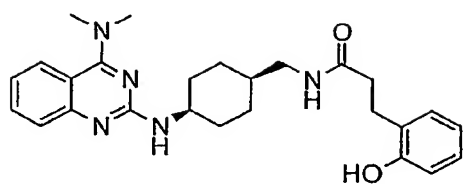


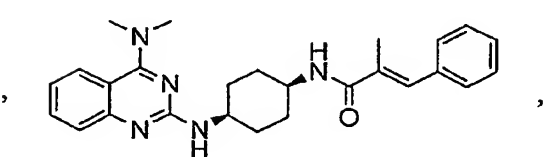
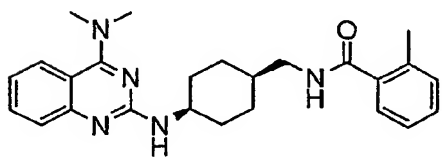
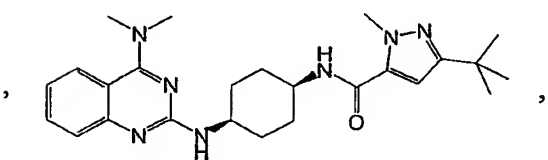
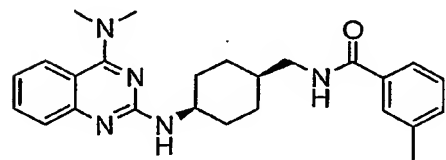
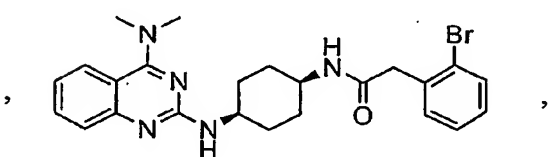
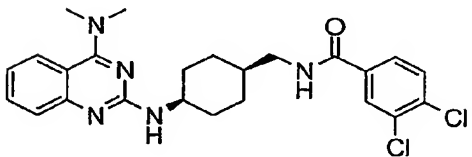
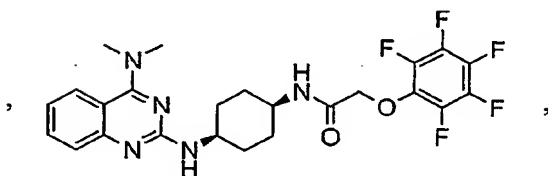
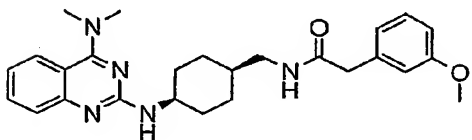
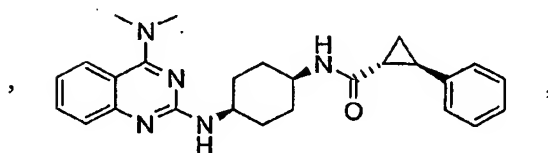
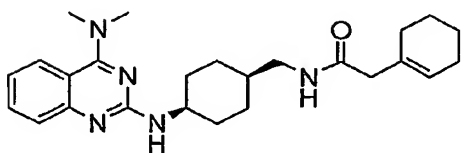
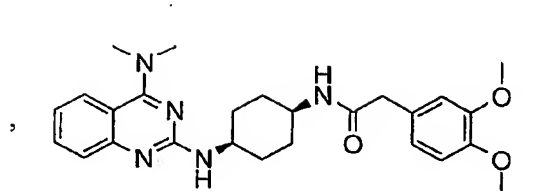
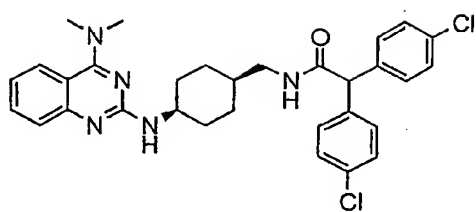


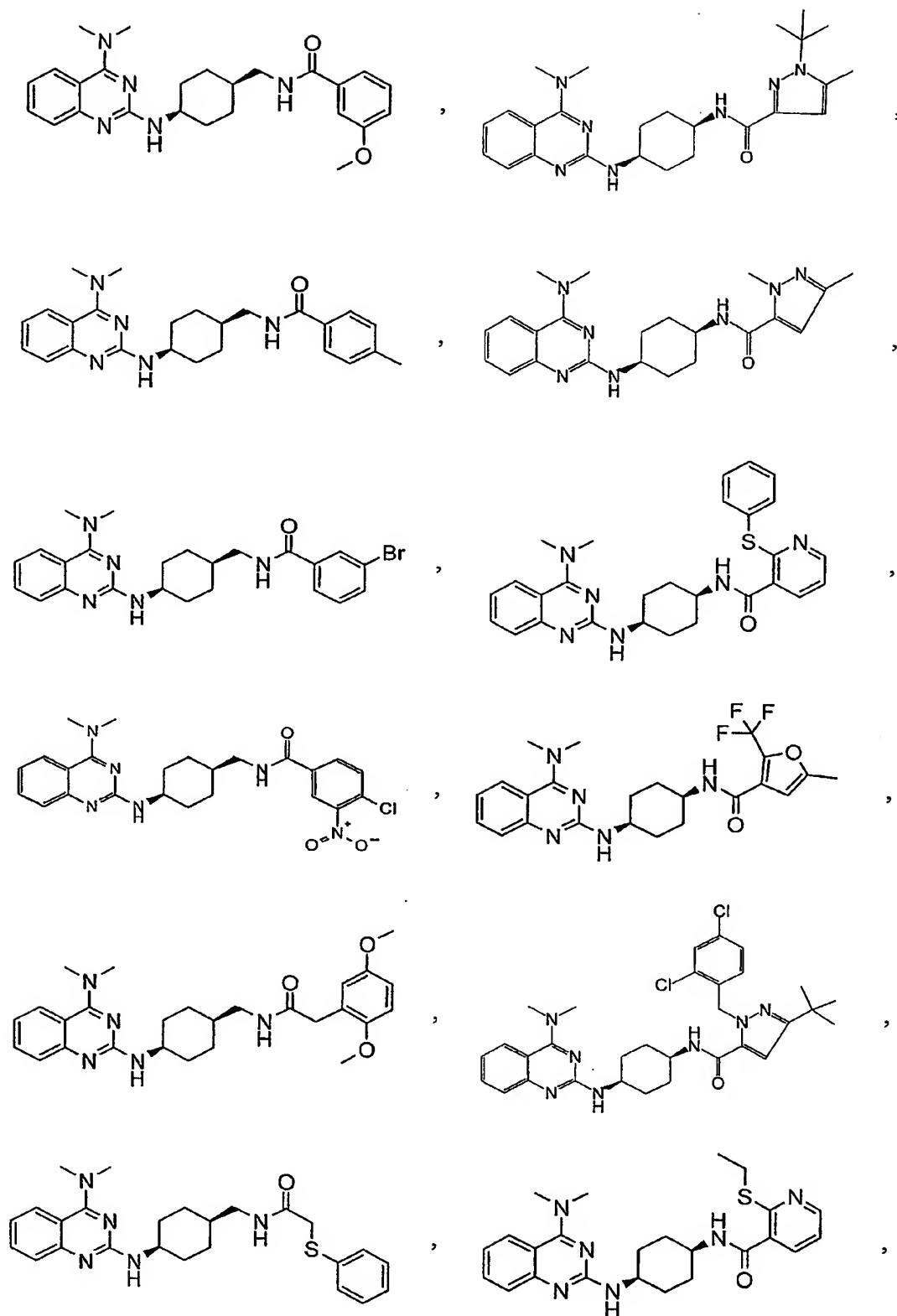


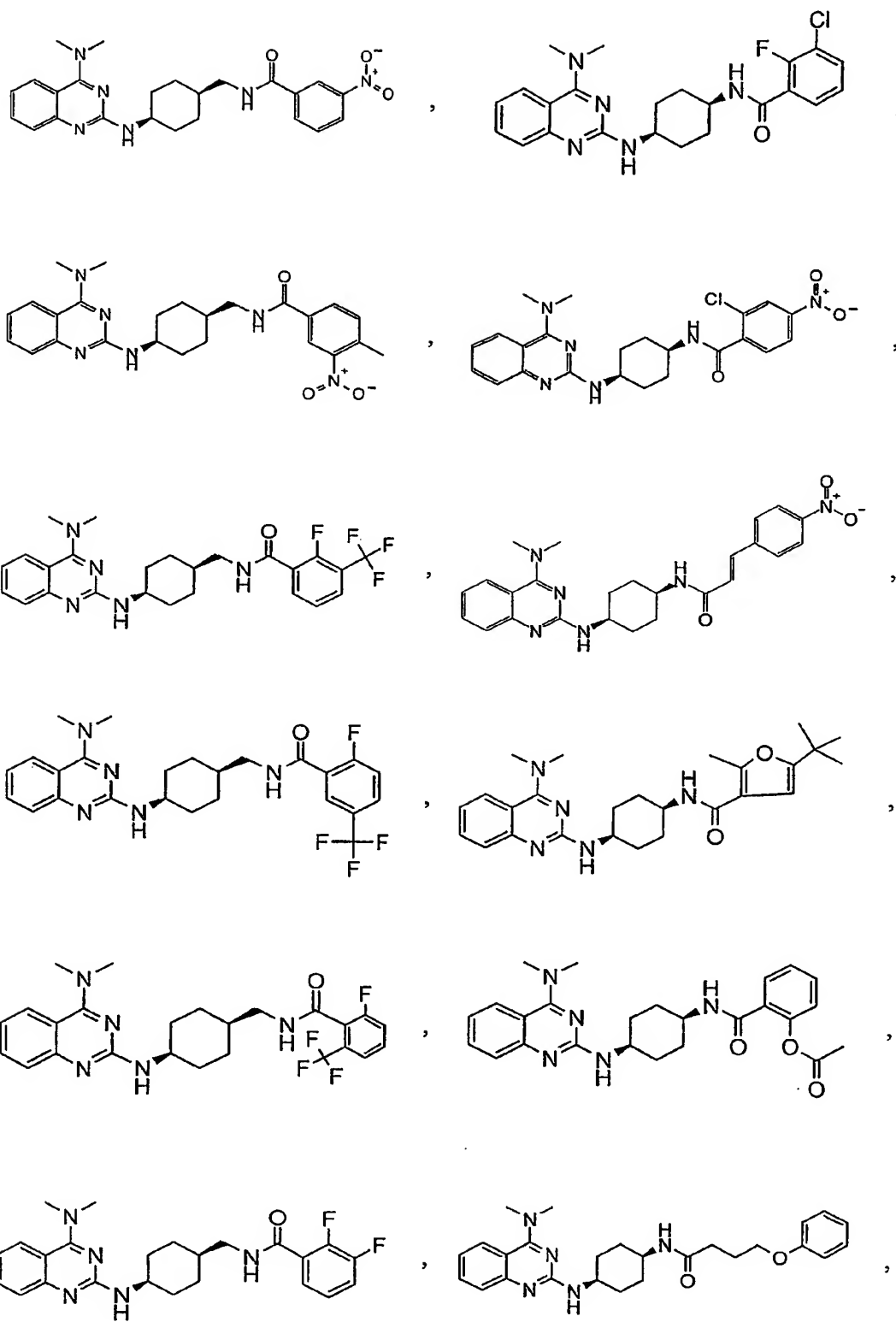


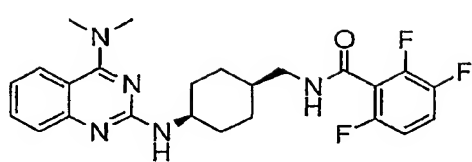




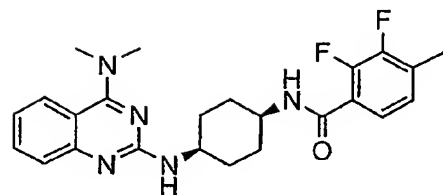




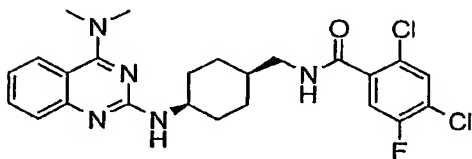




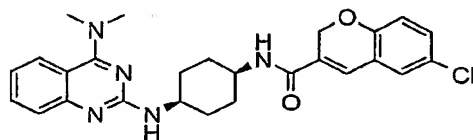
,



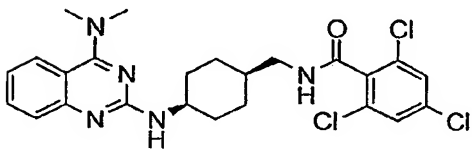
,



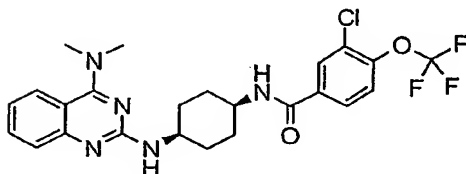
,



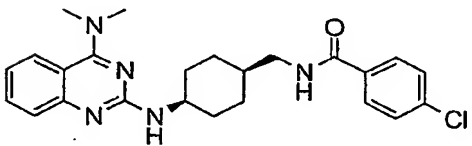
,



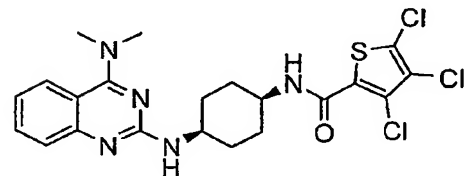
,



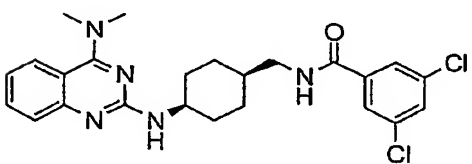
,



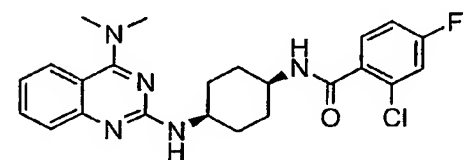
,



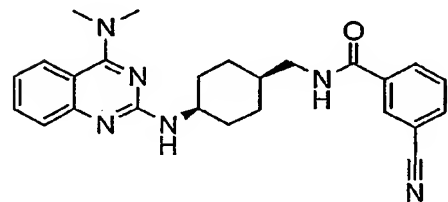
,



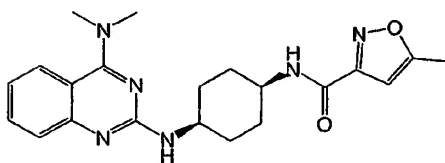
,



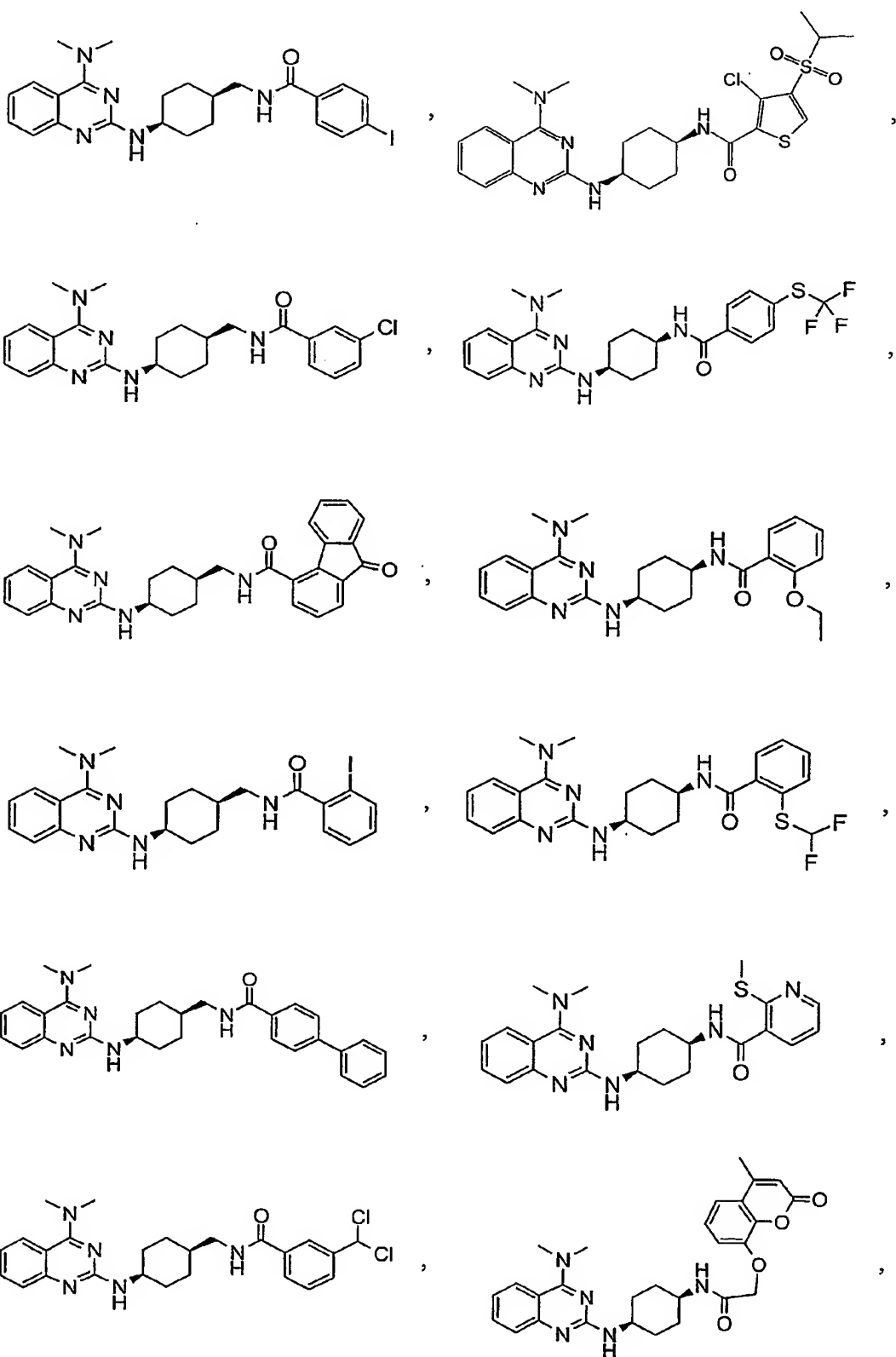
,

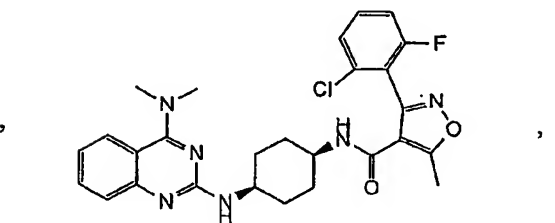
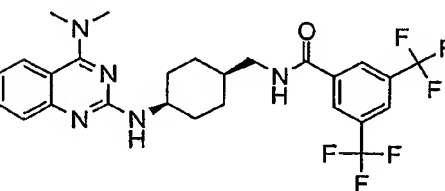
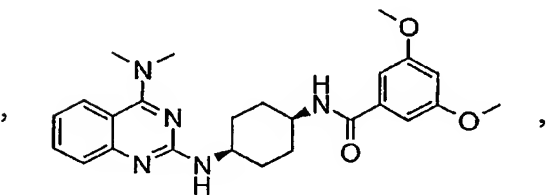
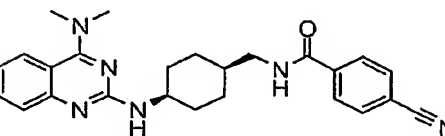
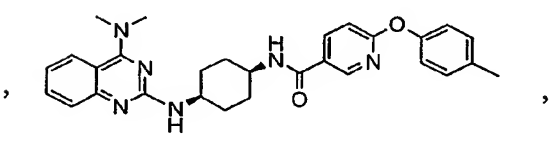
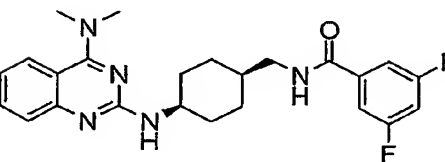
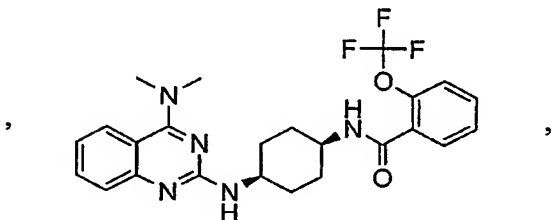
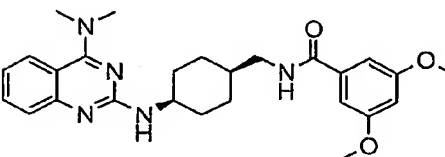
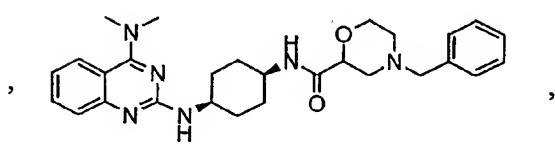
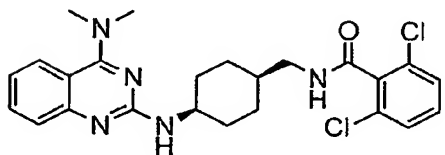
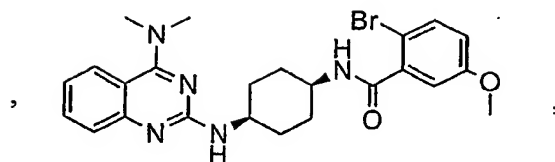
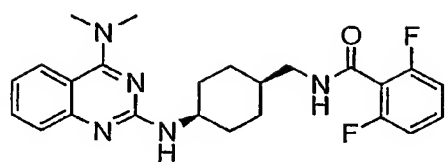


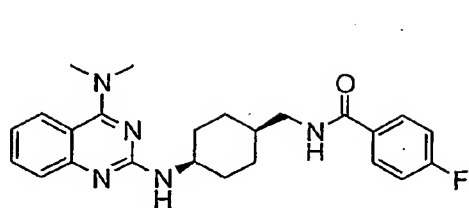
,



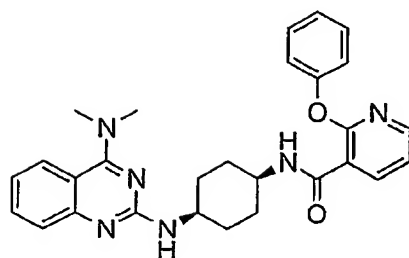
,



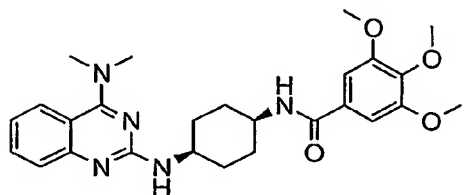




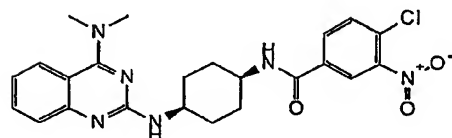
,



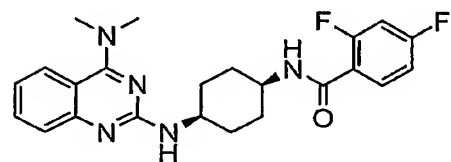
,



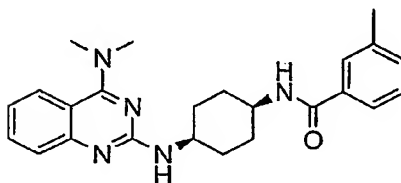
,



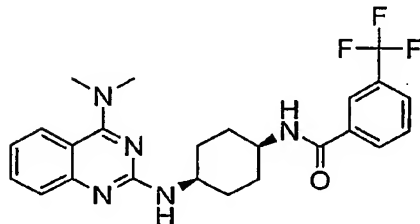
,



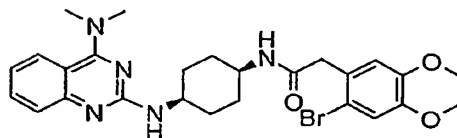
,



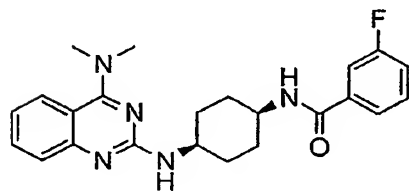
,



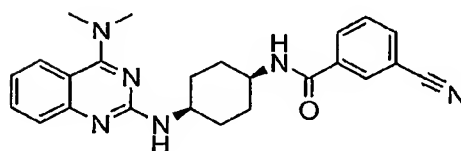
,



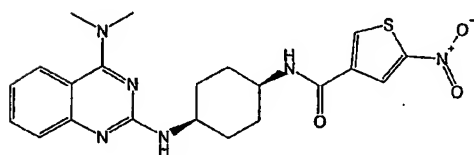
,



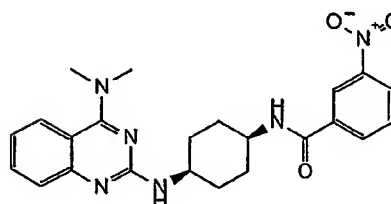
,



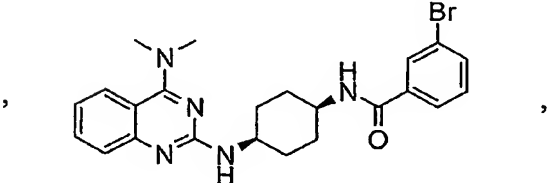
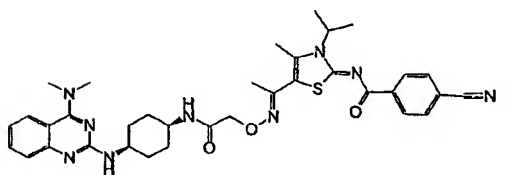
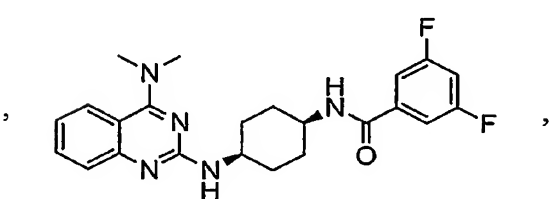
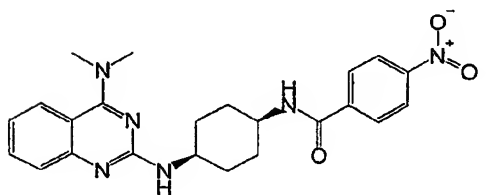
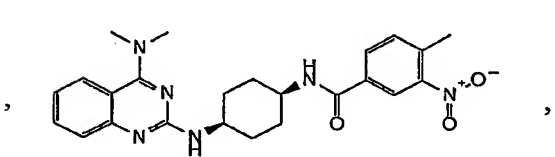
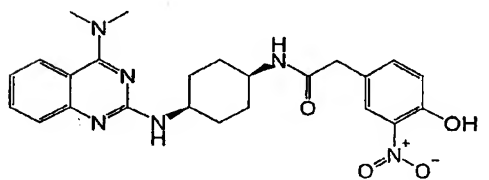
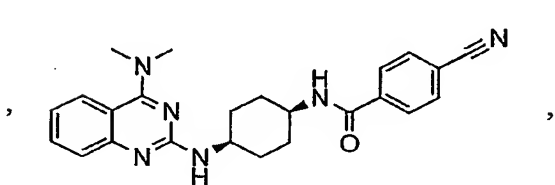
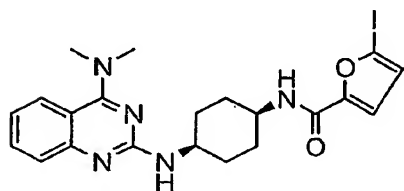
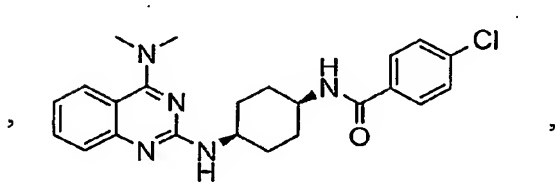
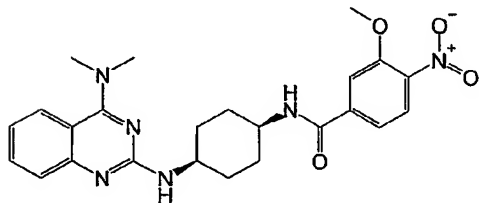
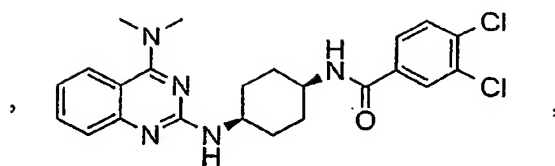
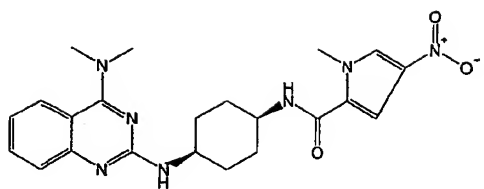
,

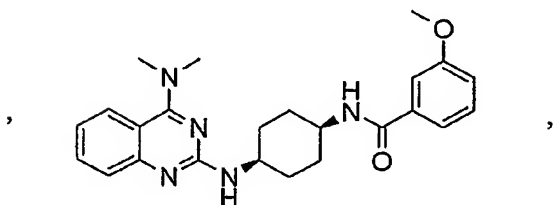
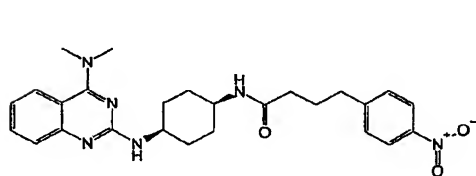
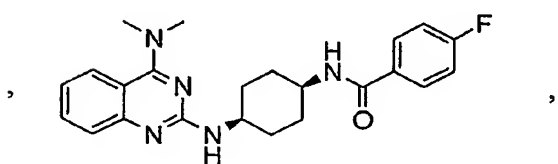
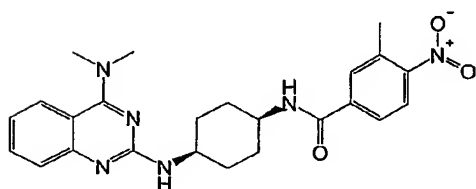
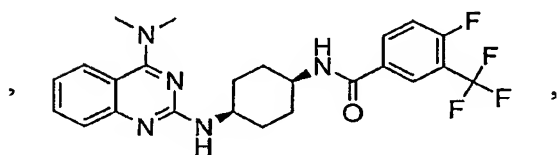
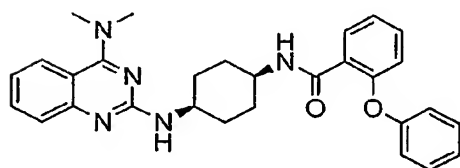
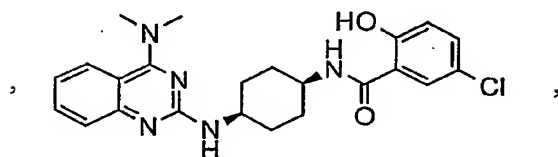
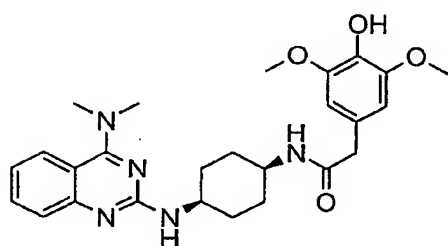
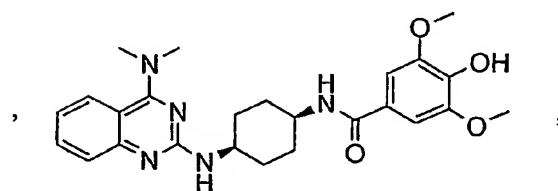
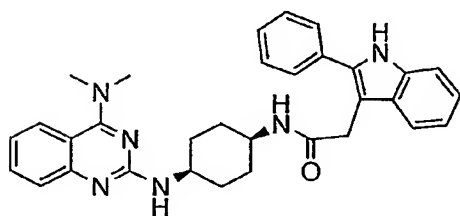
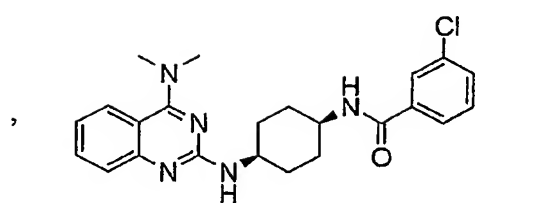
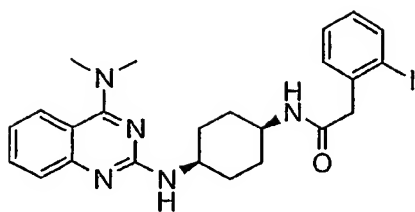


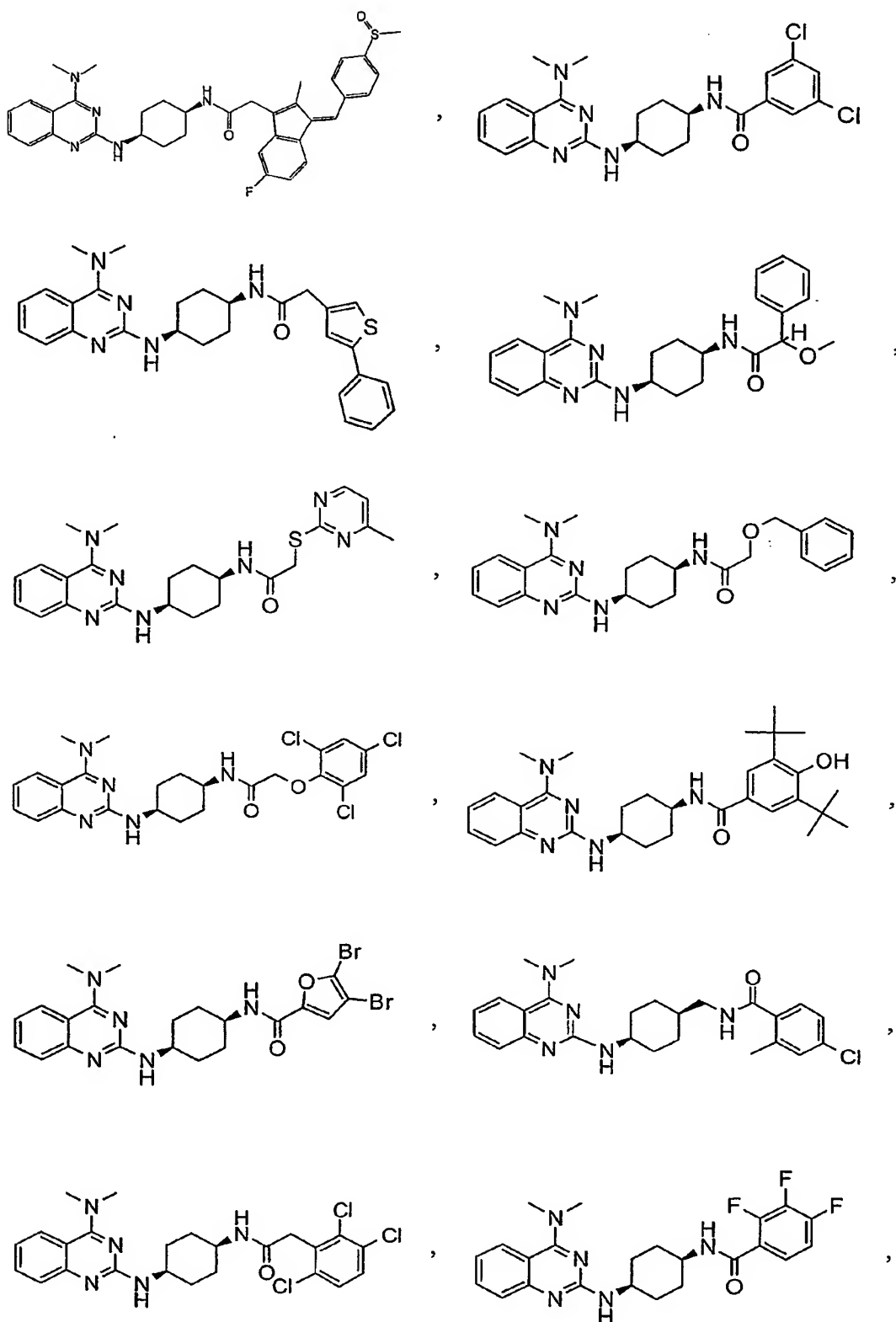
,

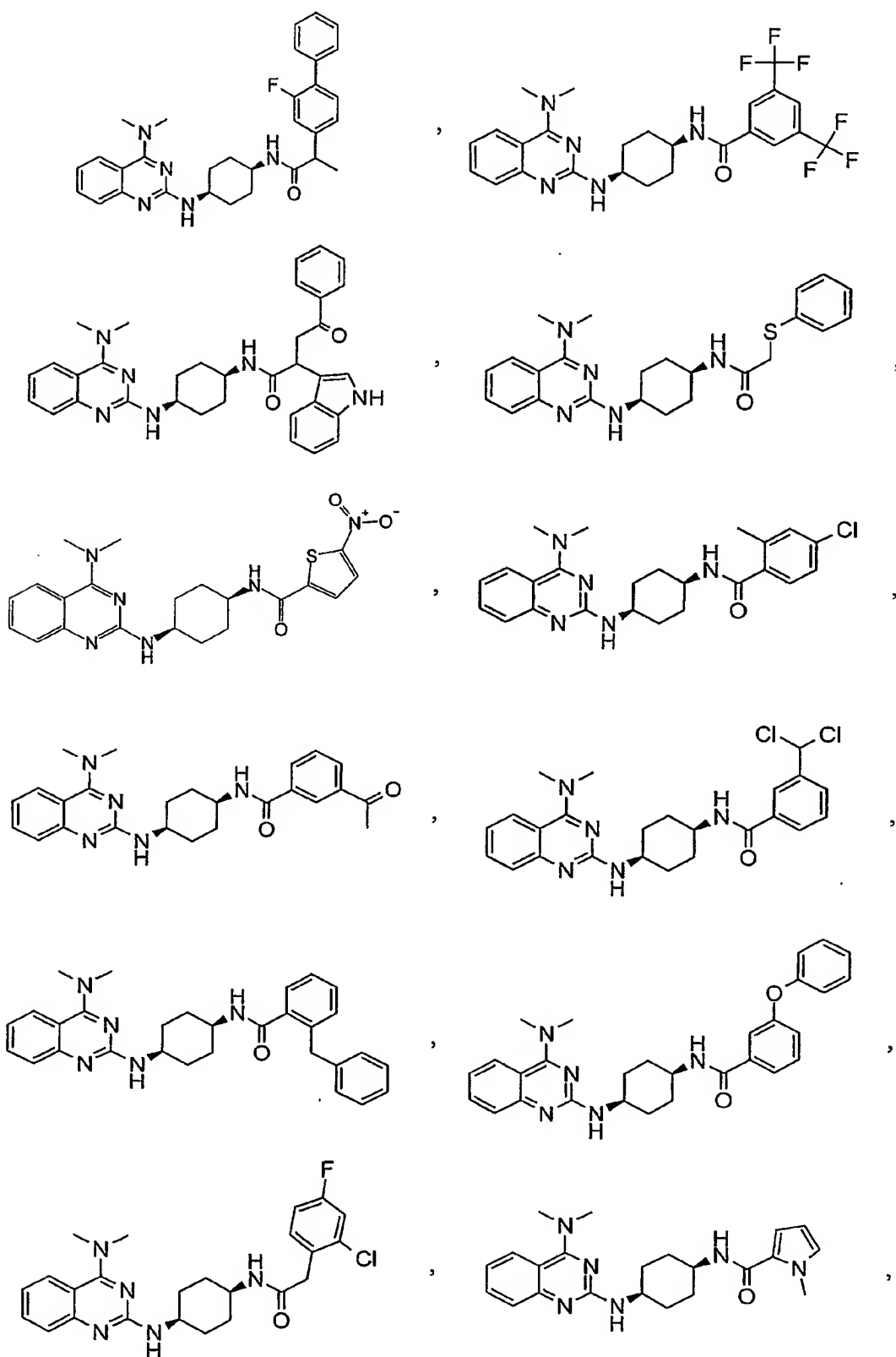


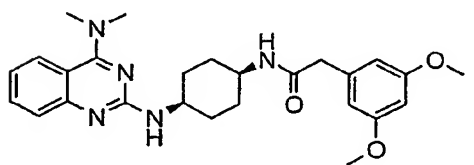
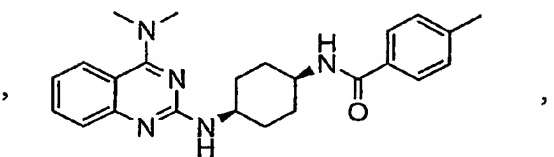
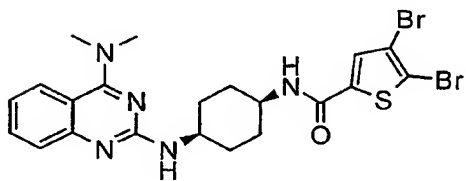
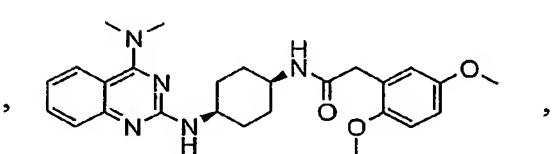
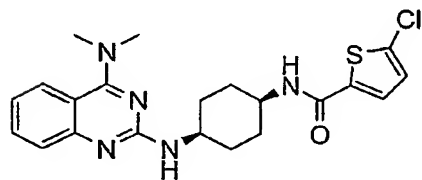
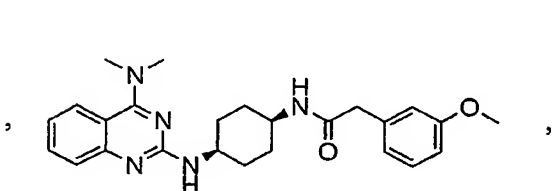
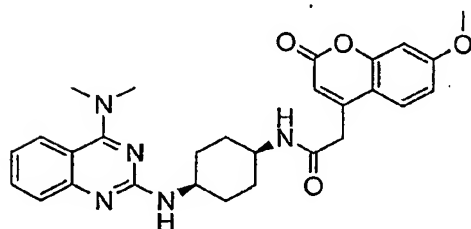
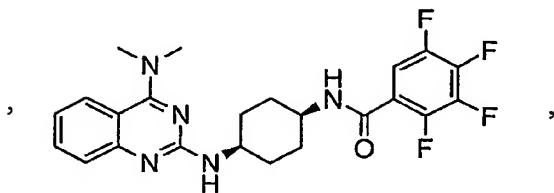
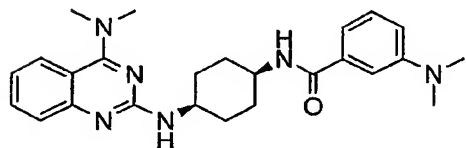
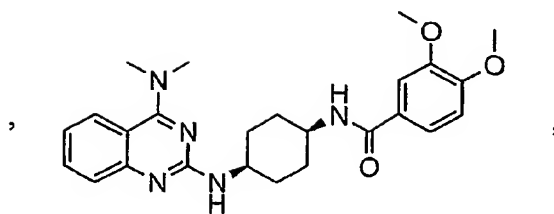
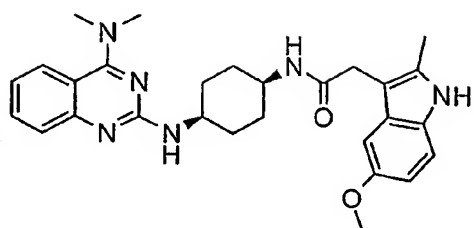
,

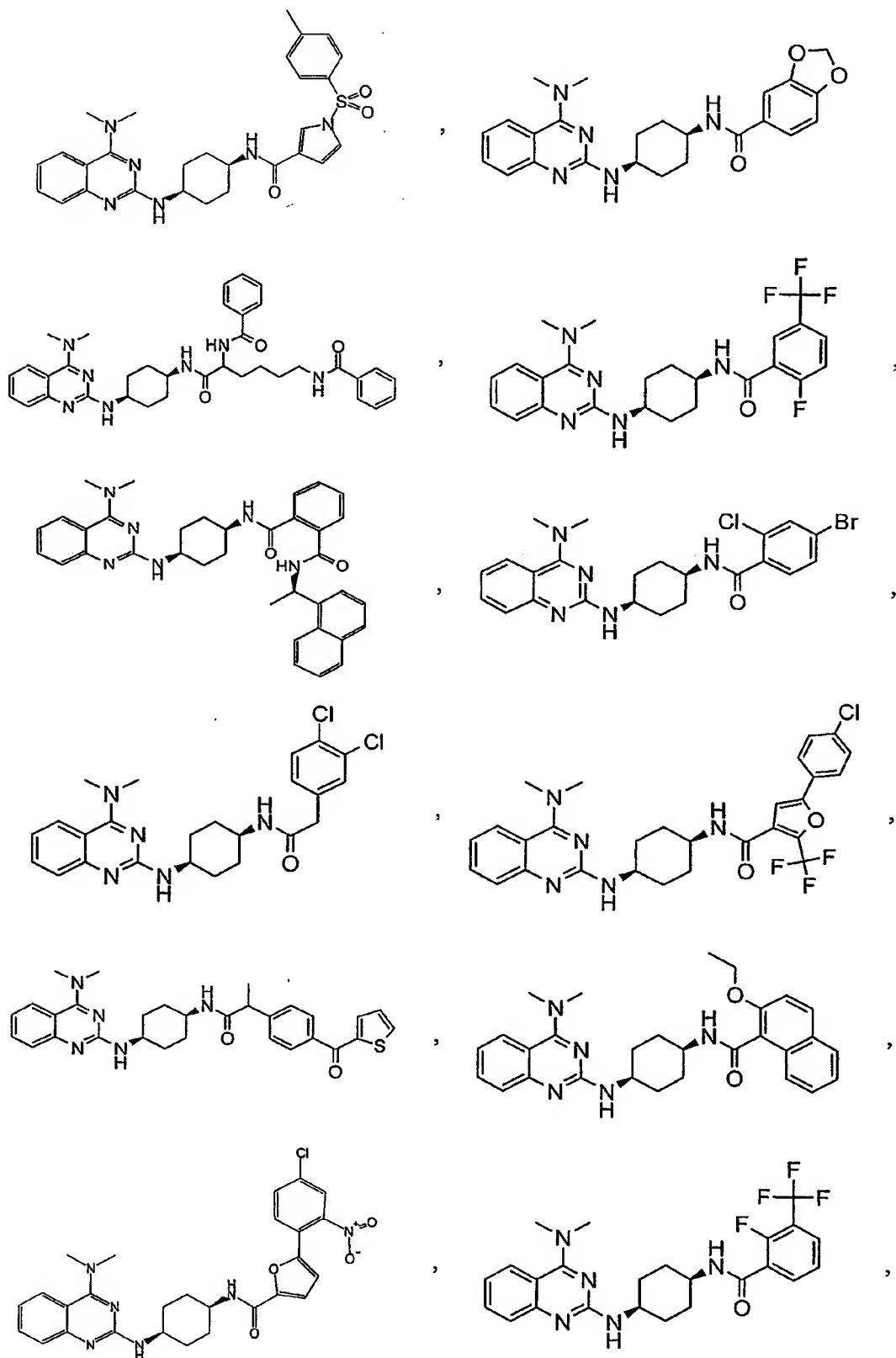


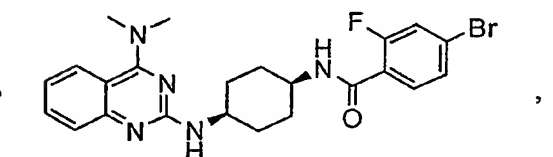
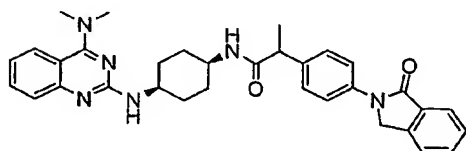
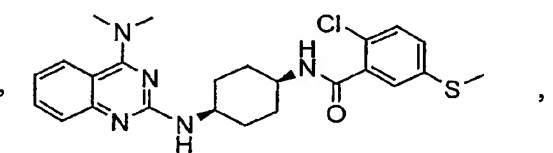
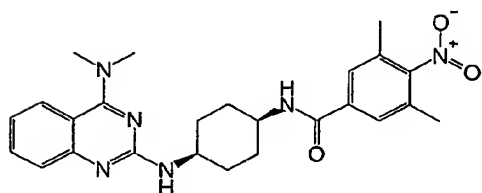
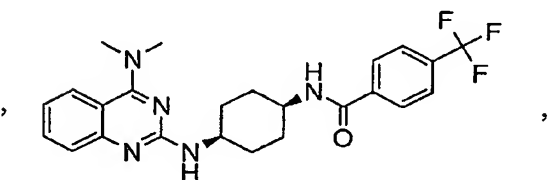
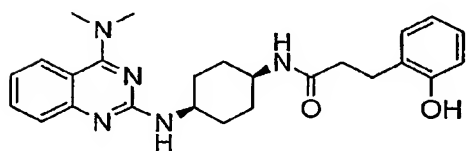
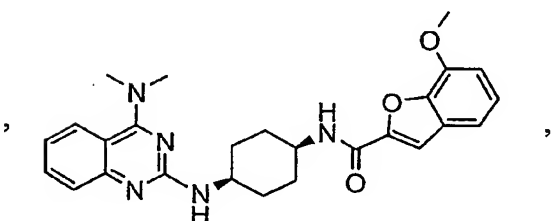
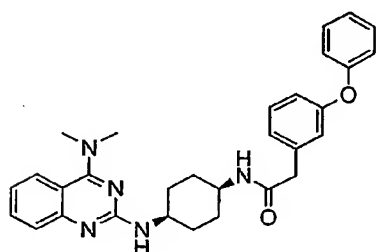
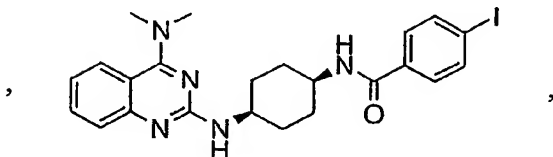
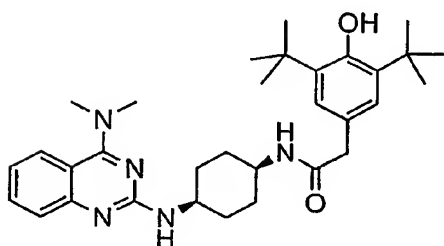
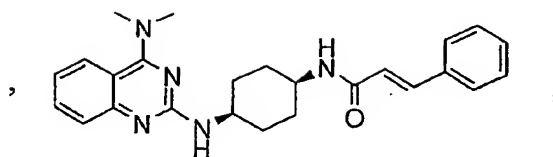
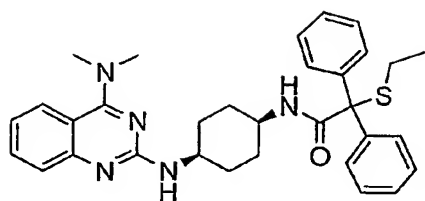


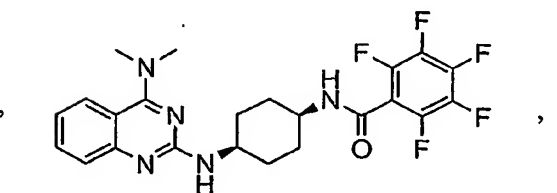
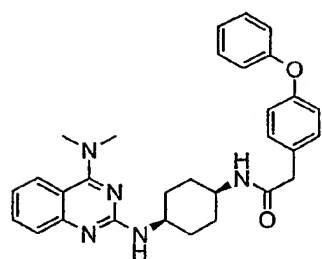
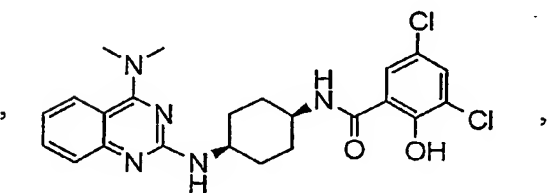
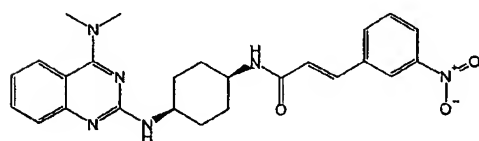
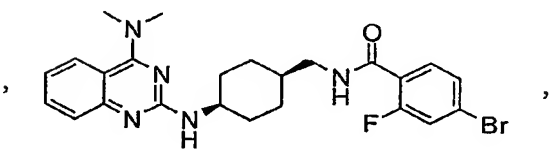
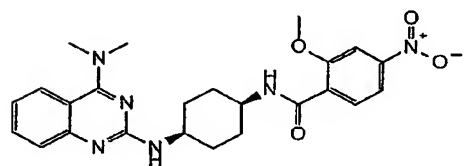
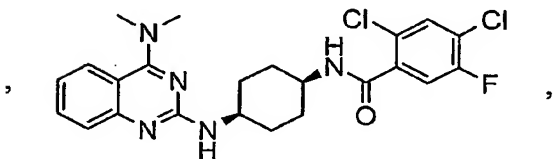
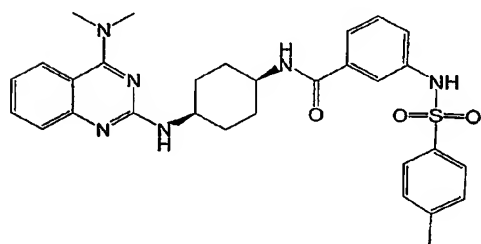
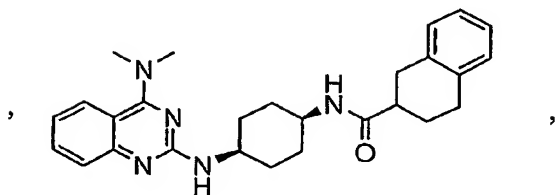
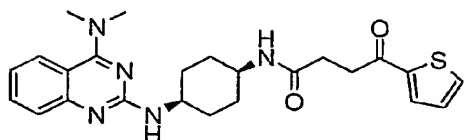
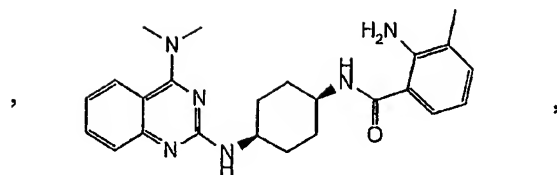
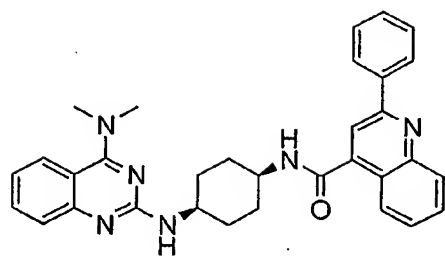


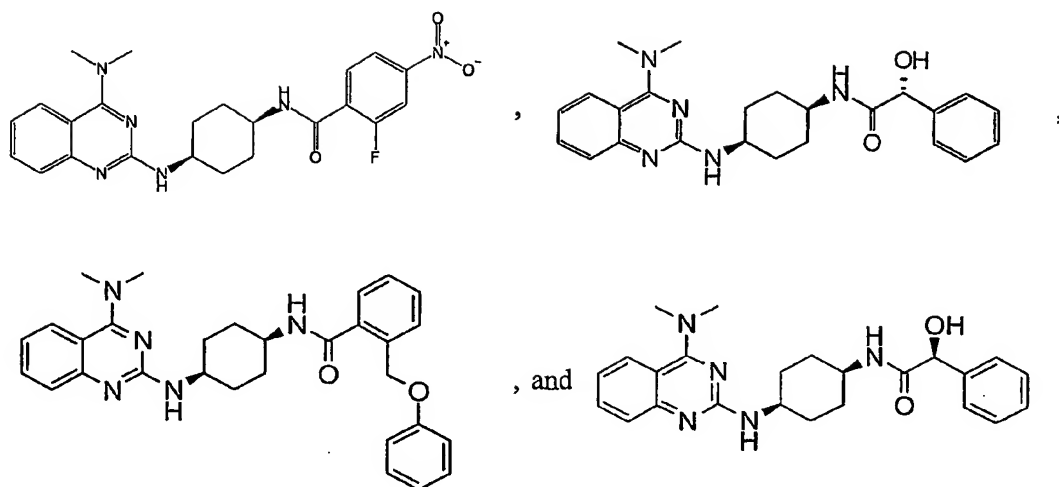












; or, in case of, a salt thereof.

7. A compound according to claim 3, wherein

R₁ represents

(i) C₁-C₁₀ alkyl,

C₁-C₁₀ alkyl substituted by substituent(s) independently selected from

•C₅-C₆ cycloalkyl,

•carbocyclic aryl,

•heterocyclyl,

(ii) C₃-C₆ cycloalkyl,

(iii) carbocyclic aryl,

(iv) or heterocyclyl;

L is selected from Formula XX - XXII;

wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 1,3-dioxo-isoindolyl, 1*H*-indolyl, 1-oxo-3*H*-isobenzofuranyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[b][1,4]dioxepinyl, 4-oxo-3,4-dihydro-phthalazinyl, 9,10,10-trioxo-thioxanthenyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, morpholino, oxolanyl, piperidyl, pyridyl, quinoxalyl, thienyl, quinolyl, or benzothiazolyl; or a salt thereof.

8. A compound according to claim 7, wherein

R₁ represents

(i) C₁-C₄ alkyl,

C₁-C₄ alkyl substituted by substituent(s) independently selected from

•cyclopentyl,

•carbocyclic aryl,

•heterocyclyl,

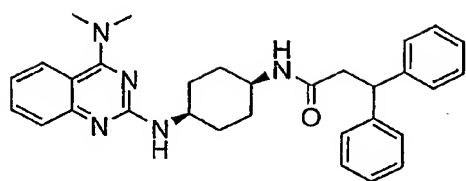
(ii) carbocyclic aryl,

(iii) or heterocyclyl;

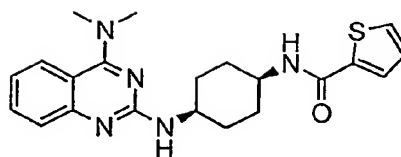
wherein carbocyclic aryl is phenyl, naphthyl, anthranyl, or biphenyl;

heterocyclyl is 9*H*-xanthenyl, benzo[1,3]dioxolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, thienyl, 1*H*-indolyl, quinoxalyl, quinolyl, or benzothiazolyl; or a salt thereof.

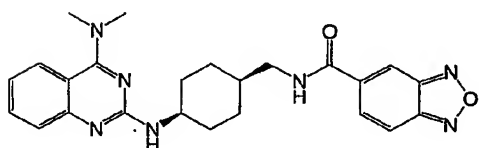
9. A compound according to claim 8 of Formua I thereof selected from the group consisting of



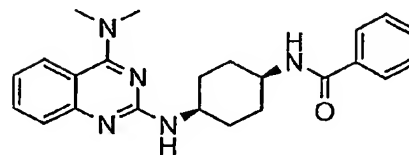
,



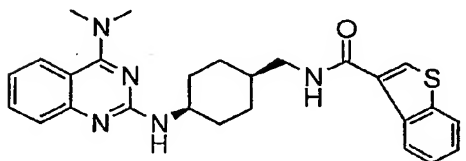
,



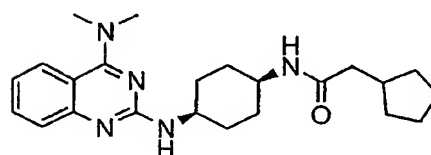
,



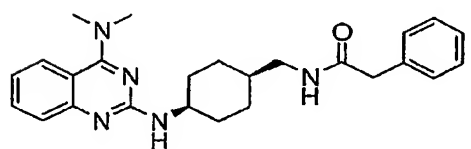
,



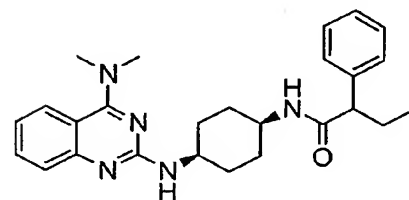
,



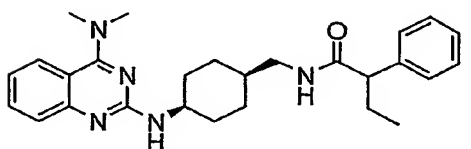
,



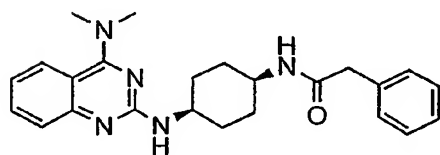
,



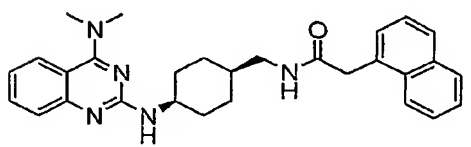
,



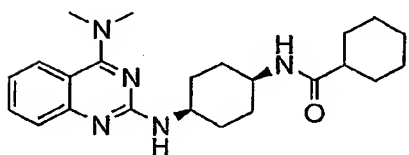
,



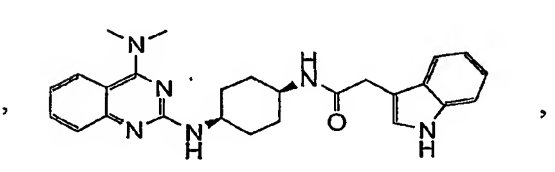
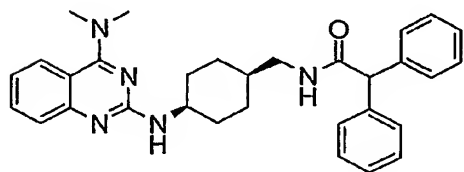
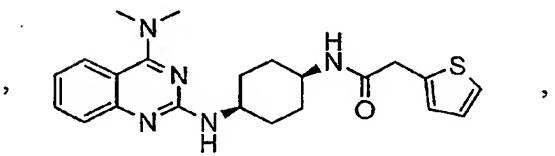
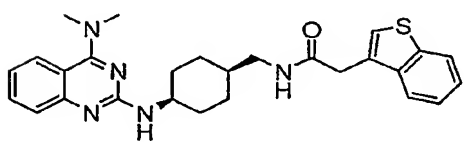
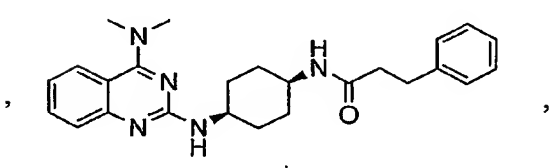
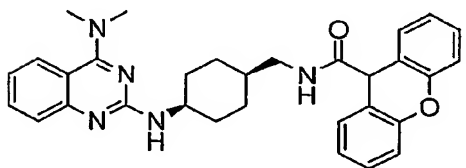
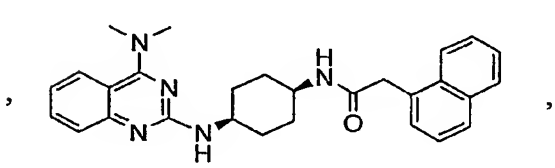
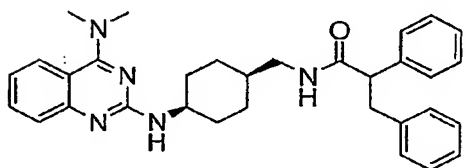
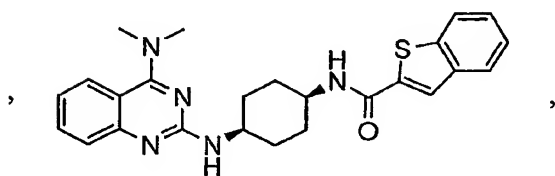
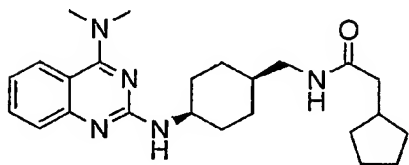
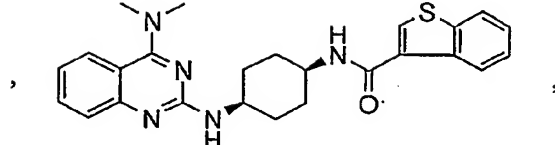
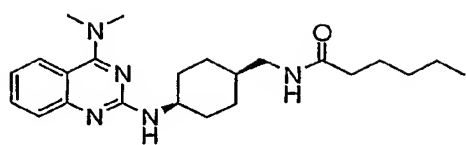
,

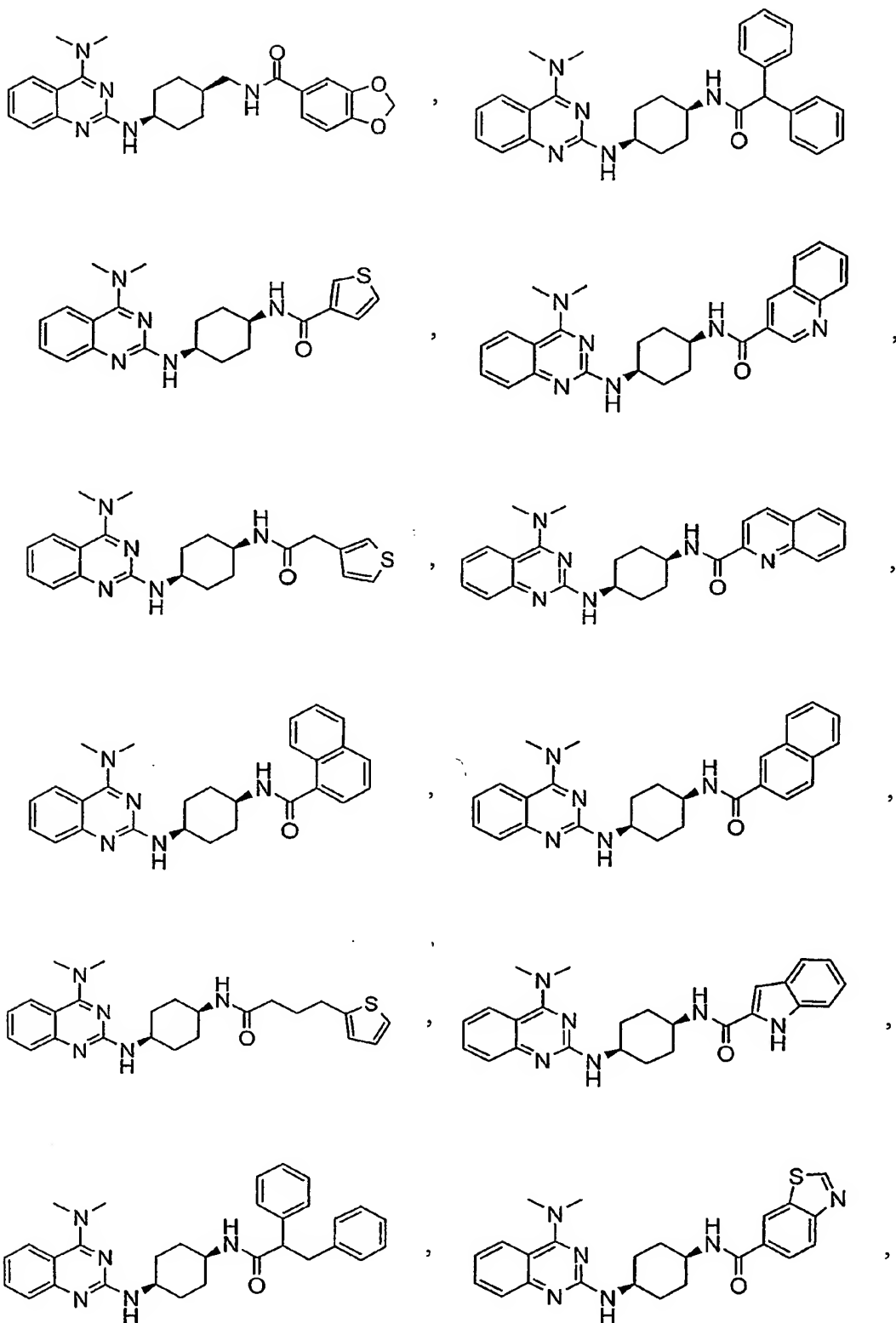


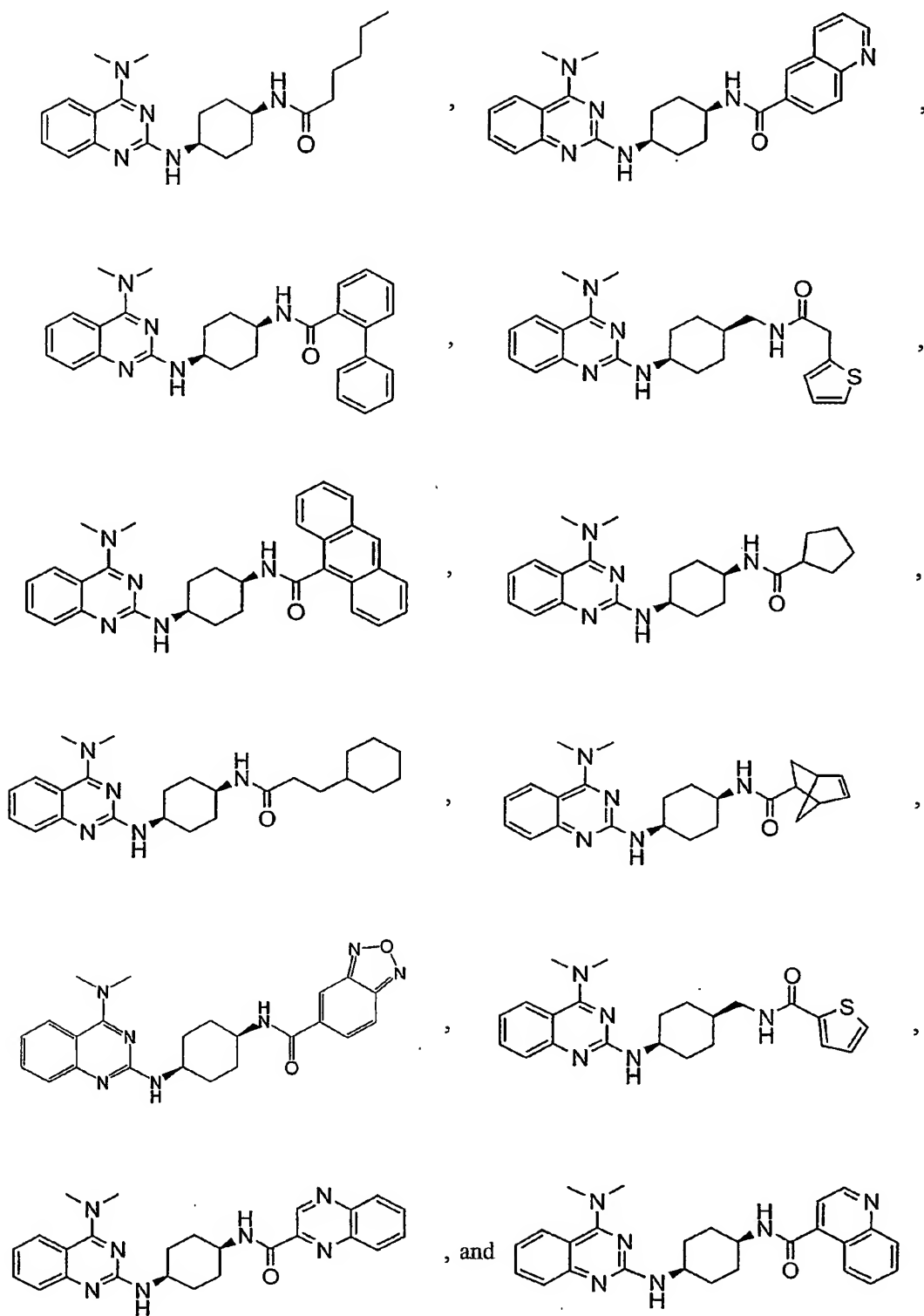
,



,







; or, in case of, a salt thereof.

10. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

- (i) C₁-C₁₀ alkyl,
- C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - carbocyclic aryloxy,
 - carbocyclic aryloxy substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by C₁-C₃ alkoxy,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino substituted by halogenated carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by substituent(s) independently selected from
 - cyano,
 - carbocyclic aryl,
 - heterocyclyl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkyl,
 - C₁-C₃ alkylcarbonylamino,
 - C₁-C₄ alkoxycarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by substituent(s) independently selected from
 - nitro,
 - C₁-C₃ alkyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - C₁-C₃ alkylthio substituted by substituent(s) independently selected from
 - mono- or di-carbocyclic arylamino,
 - halogenated mono- or di-carbocyclic arylamino,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - carbocyclic arylthio,
 - carbocyclic arylthio substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
- carbocyclic arylsulfonyl,
- halogenated carbocyclic arylsulfonyl,
- heterocyclylthio,
- C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by C₁-C₃ alkyl,
- carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl substituted C₁-C₃ alkylsulfinyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,

- hydroxy,
- nitro,
- C₁-C₄ alkyl,
- C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - carbocyclic aryl,
 - carbocyclic aryloxy,
 - C₁-C₃ alkoxycarbonyl,
 - mono- or di-C₁-C₃ alkylamino,
 - C₁-C₃ alkylthio,
 - halogenated C₁-C₃ alkylthio,
 - C₁-C₃ alkylsulfonyl,
 - C₃-C₆ cycloalkyl,
 - carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkoxy,

- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- (ii) C₂-C₈ alkenyl,
- C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - C₁-C₃ alkoxy,
 - halogenated C₁-C₃ alkoxy,
 - heterocyclyl,
 - heterocyclyl substituted by nitro,
- (iii) C₂-C₄ alkynyl,
- C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) C₃-C₆ cycloalkyl,
- C₃-C₆ cycloalkyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by substituent(s) independently selected from
 - hydroxy,
 - oxo,
 - carbocyclic aryl,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - carbocyclic aryl,
- (v) C₃-C₆ cycloalkenyl,
- C₃-C₆ cycloalkenyl substituted by C₁-C₃ alkyl,
- (vi) carbocyclyl,
- carbocyclyl substituted by substituent(s) independently selected from

- hydroxy,
- nitro,
- (vii) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₉ alkyl,
 - C₁-C₉ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - oxo,
 - C₁-C₃ alkoxy,
 - carbocyclic aryloxy,
 - mono- or di-C₁-C₃ alkylamino-N-oxy,
 - mono- or di-C₁-C₃ alkylamino,
 - mono- or di-C₁-C₃ alkylamino substituted by carbocyclic aryl,
 - mono- or di-carbocyclic arylamino,
 - mono- or di-carbocyclic arylamino substituted by C₁-C₃ alkoxy,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
 - heterocyclyl,
 - heterocyclyl substituted by C₁-C₃ alkyl,
 - C₂-C₃ alkenyl,
 - C₂-C₃ alkenyl substituted by carbocyclic aryl,
 - C₁-C₉ alkoxy,
 - C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - hydroxy,
 - halogen,
 - carboxy,
 - mono- or di-C₁-C₃ alkylamino,

- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- halogen,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₂-C₃ alkenyloxy,
- C₁-C₃ alkylcarbonyloxy,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by substituent(s) independently selected from
- halogen,
- C₁-C₄ alkyl,
- halogenated C₁-C₄ alkyl,
- C₁-C₃ alkoxy,
- heterocyclyloxy,
- heterocyclyloxy substituted by substituent(s) independently selected from
- halogen,
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- (carbocyclic aryl)S(O)₂O,
- carboxy,
- C₁-C₃ alkoxycarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl,
- mono- or di-C₁-C₃ alkylaminocarbonyl substituted by carbocyclic aryl,
- amino,
- mono- or di-C₁-C₄ alkylamino,
- mono- or di-C₁-C₄ alkylamino substituted by cyano,
- mono- or di-carbocyclic arylamino,
- C₁-C₃ alkylcarbonylamino,

- carbocyclic arylsulfonylamino,
- carbocyclic arylsulfonylamino substituted by C₁-C₃ alkyl,
- (carbocyclic aryl)NHC(O)NH,
- (carbocyclic aryl)NHC(O)NH substituted by C₁-C₃ alkoxy,
- (carbocyclic aryl)NHC(O)NH substituted by halogenated C₁-C₃ alkoxy,
- C₁-C₃ alkylthio,
- halogenated C₁-C₃ alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C₁-C₃ alkyl,
- heterocyclylthio,
- C₁-C₃ alkylsulfonyl,
- mono- or di-C₁-C₃ alkylaminosulfonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - C₁-C₇ alkyl,
 - halogenated C₁-C₇ alkyl,
 - heterocyclyl,
 - heterocyclyl substituted by substituent(s) independently selected from
 - C₁-C₃ alkyl,
 - carbocyclic aryl,
 - halogenated carbocyclic aryl,
- (viii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,

- oxo,
- C₁-C₃ alkylcarbonyloxy,
- C₁-C₃ alkoxycarbonyl,
- C₁-C₃ alkylthio,
- C₁-C₃ alkylthio substituted by carbocyclic aryl,
- C₁-C₃ alkylthio substituted by halogenated carbocyclic aryl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- heterocyclyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- carbocyclic aryloxy substituted by C₁-C₃ alkyl,
- mono- or di-C₁-C₃ alkylamino,
- C₁-C₄ alkylcarbonylamino,
- C₁-C₃ alkylthio,
- carbocyclic arylthio,
- halogenated carbocyclic arylthio,
- carbocyclic arylthio substituted by C₁-C₃ alkoxycarbonyl,
- heterocyclylthio,
- heterocyclylthio substituted by C₁-C₃ alkyl,
- C₁-C₃ alkylsulfonyl,
- carbocyclic arylsulfonyl,
- carbocyclic arylsulfonyl substituted by C₁-C₄ alkyl,
- C₁-C₃ alkoxycarbonyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
- halogen,
- nitro,
- C₁-C₃ alkyl,

- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- halogenated C₁-C₃ alkoxy,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
- C₁-C₃ alkyl,
- halogenated C₁-C₃ alkyl,
- C₁-C₃ alkoxy,
- C₁-C₃ alkoxycarbonyl;

Y is -(CH₂)_m, m is 0 or 1;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;
 carbocyclyl is 9*H*-fluorenyl, 9-oxo-fluorenyl, acenaphthyl, anthraquinonyl, indanyl, or indenyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3,4-thiadiazolyl, 1,3-dioxo-isindolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolo[2,3-*c*]pyridyl, 1*H*-pyrrolyl, 2,2',5',2"-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-1-oxo-isindolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 2,3-dihydro-benzofuryl, 2,4-dihydro-3-oxo-pyrazolyl, 2*H*-benzopyranyl, 2-oxo-pyrrolidinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 3,4-dihydro-2*H*-benzo[*b*][1,4]dioxepinyl, 4*H*-benzo[1,3]dioxinyl, 4*H*-benzopyranyl, 4-oxo-1,5,6,7-tetrahydro-indolyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, azetidiny, benzimidazolyl, benzo[1,3]dioxolyl, benzo[*b*]thienyl, benzofuryl, benzothiazolyl, furyl, imidazo[2,1-*b*]thiazolyl, imidazolyl, isoxazolyl, morpholino, morpholinyl, oxolanyl, piperazyl, piperidyl, pyrazolo[5,1-*b*]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, pyrrolidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, or thiolanyl;

halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

11. A compound according to claim 10, wherein

R₁ represents

- (i) C₁-C₁₀ alkyl substituted by substituent(s) independently selected from
- methoxy,
- methoxy substituted by carbocyclic aryl,

- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-C₁-C₂ alkylamino substituted by cyano,
- mono- or di-C₁-C₂ alkylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - C₁-C₂ alkoxy,
 - halogenated C₁-C₂ alkoxy,
 - heterocyclyl substituted by carbocyclic aryl,
- (ii) C₂-C₈ alkenyl substituted by substituent(s) independently selected from
 - methoxy substituted by carbocyclic aryl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by methoxy,
- (iii) C₂-C₄ alkynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₉ alkyl,
 - halogenated C₁-C₉ alkyl,

- C₁-C₉ alkoxy,
- C₁-C₉ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - halogenated carbocyclic aryl,
- propenyloxy,
- methylamino,
- di-C₁-C₂ alkylamino,
- di-C₁-C₂ alkylamino substituted by cyano,
- methylthio,
- halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - methoxy,
 - C₁-C₂ alkoxycarbonyl,
 - carbocyclic arylthio substituted by methoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - halogenated methyl,
- heterocyclyl;

R₂ is methylamino or dimethylamino;

L is selected from Formula Va, VIIIa, or IXa;

wherein carbocyclic aryl is phenyl, naphthyl, biphenyl, or phenanthryl;

carbocyclyl is 9*H*-fluorenyl, acenaphthyl, or anthraquinonyl;

heterocyclyl is 1,2,3-thiadiazolyl, 1,2,3-triazolyl, 1,2-dihydro-3-oxo-pyrazolyl, 1,3-dioxolanyl, 1*H*-indolyl, 1*H*-pyrrolyl, 2,2',5',2''-terthiophenyl, 2,2'-bithiophenyl, 2,3-dihydro-benzo[1,4]dioxinyl, 3,4-dihydro-2*H*-benzo[1,4]oxazinyl, 4-oxo-benzopyranyl, 9*H*-carbazolyl, 9*H*-xanthenyl, benzimidazolyl, benzo[1,3]dioxolyl, benzo[b]thienyl, benzofuryl,

benzothiazolyl, furyl, imidazolyl, isoxazolyl, oxolanyl, pyrazolo[5,1-b]thiazolyl, pyrazolyl, pyridyl, pyrimidyl, quinolyl, quinoxalyl, thiazolidyl, thiazolyl, thienyl, 2*H*-benzopyranyl, 4*H*-benzo[1,3]dioxinyl, azetidiny, imidazo[2,1-b]thiazolyl, morpholinyl, or 2,3-dihydro-benzofuryl;

halogen is fluoro, chloro, bromo, or iodo;
or a salt thereof.

12. A compound according to claim 11, wherein

R₁ represents

(i) C₁-C₇ alkyl substituted by substituent(s) independently selected from

- methoxy,
- methoxy substituted by carbocyclic aryl,
- carbocyclic aryloxy,
- halogenated carbocyclic aryloxy,
- mono-ethylamino substituted by cyano,
- di-methylamino substituted by carbocyclic aryl,
- mono-carbocyclic arylamino,
- mono-carbocyclic arylamino substituted by methyl,
- carbocyclic arylsulfonylamino substituted by methyl,
- carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - nitro,
 - C₁-C₄ alkyl,
 - C₁-C₄ alkyl substituted by carbocyclic aryl,
 - C₁-C₄ alkyl substituted by hydroxy,
 - methoxy,
 - halogenated methoxy,
 - heterocyclyl substituted by carbocyclic aryl,

(ii) C₂-C₇ alkenyl substituted by substituent(s) independently selected from

- methoxy substituted by carbocyclic aryl,
- carbocyclic aryl,

- carbocyclic aryl substituted by methoxy,
- (iii) butynyl substituted by carbocyclic aryl,
- (iv) cyclohexyl substituted by carbocyclic arylmethyl,
- (v) carbocyclyl,
- (vi) carbocyclic aryl,
- carbocyclic aryl substituted by substituent(s) independently selected from
 - halogen,
 - hydroxy,
 - cyano,
 - amino,
 - C₁-C₂ alkyl,
 - halogenated methyl,
 - C₁-C₃ alkoxy,
 - C₁-C₃ alkoxy substituted by substituent(s) independently selected from
 - halogen,
 - halogenated carbocyclic aryl,
 - propenyloxy,
 - di-C₁-C₂ alkylamino,
 - di-C₁-C₂ alkylamino substituted by cyano,
 - methylthio,
 - halogenated methylthio,
- (vii) heterocyclyl,
- or heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - C₁-C₃ alkyl substituted by hydroxy,
 - C₁-C₃ alkyl substituted by carbocyclic aryl,
 - methoxy,
 - ethoxycarbonyl,
 - carbocyclic arylthio substituted by methoxycarbonyl,
 - carbocyclic aryl,
 - carbocyclic aryl substituted by substituent(s) independently selected from

- halogen,
- halogenated methyl,
- heterocyclyl;

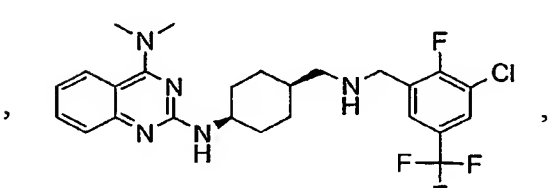
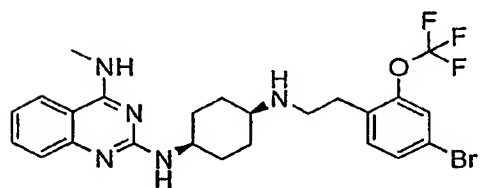
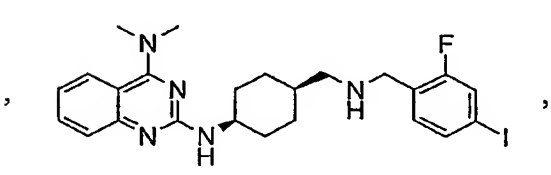
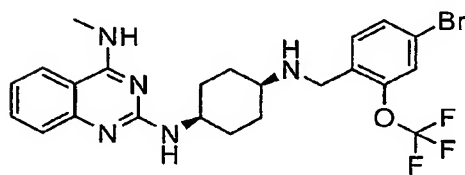
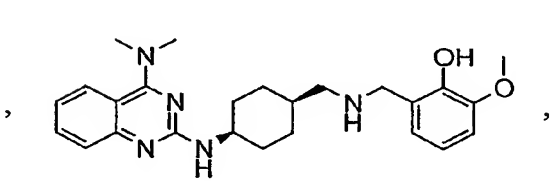
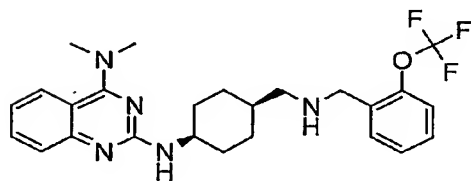
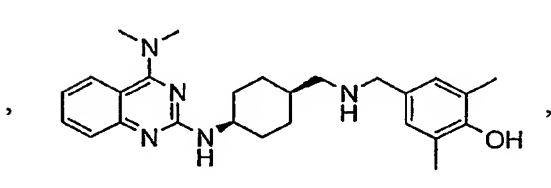
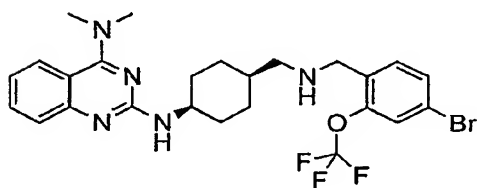
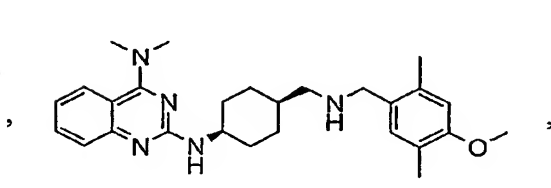
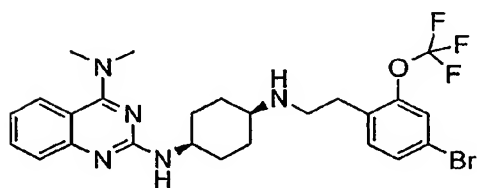
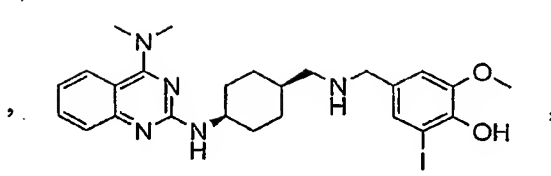
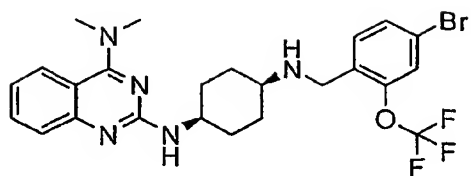
L is selected from Formula XX - XXII;

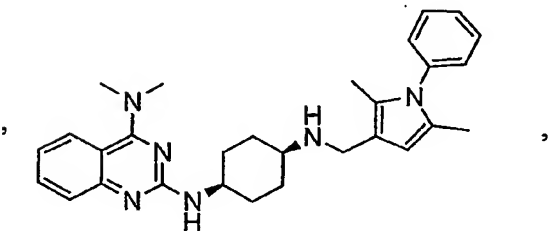
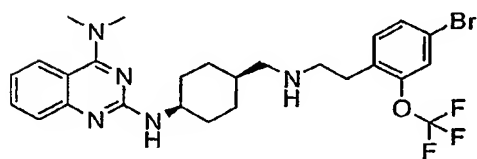
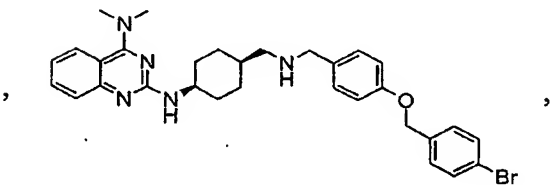
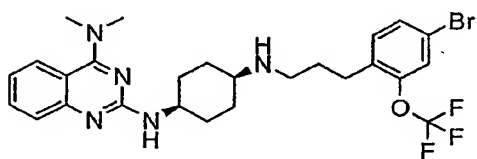
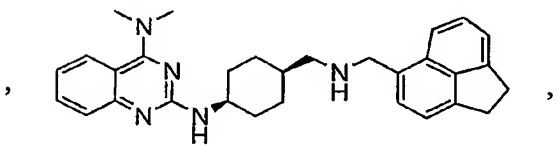
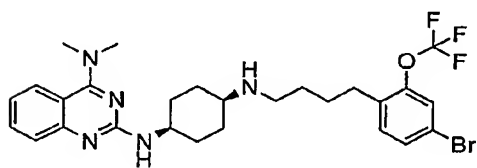
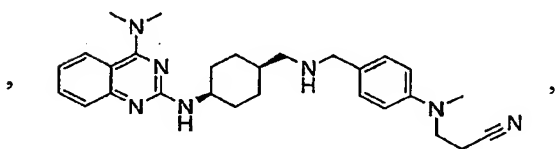
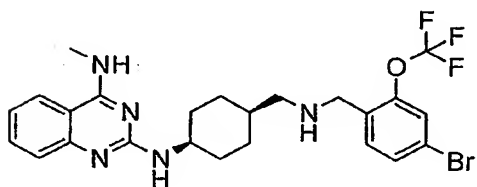
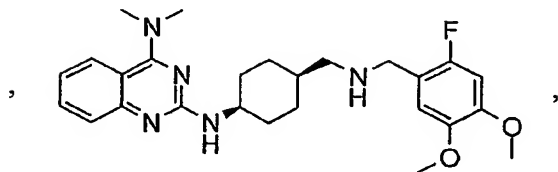
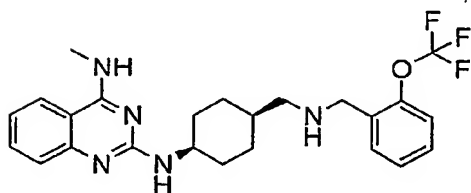
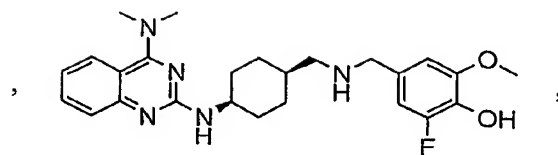
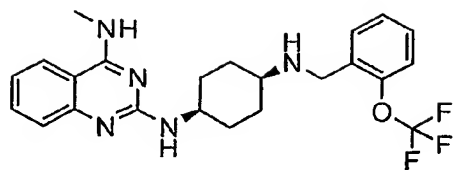
wherein carbocyclic aryl is phenyl, **naphthyl**, or biphenyl;

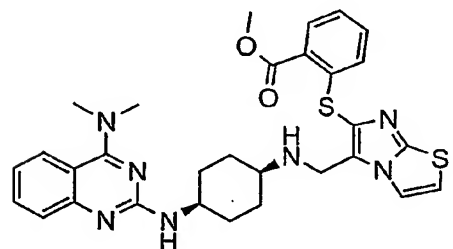
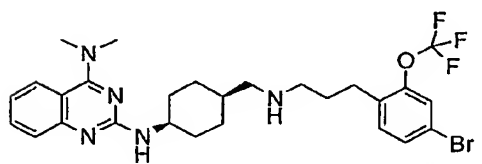
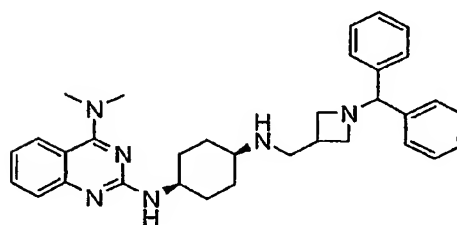
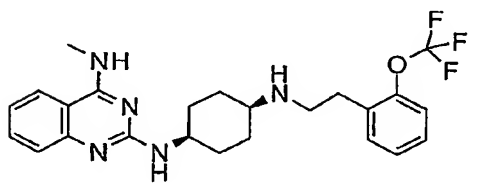
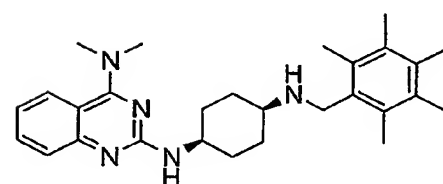
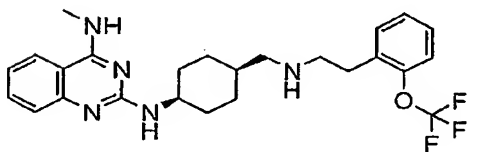
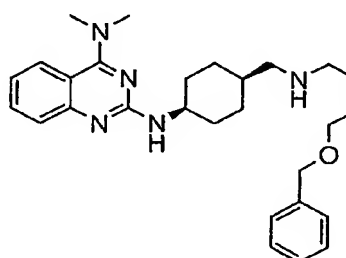
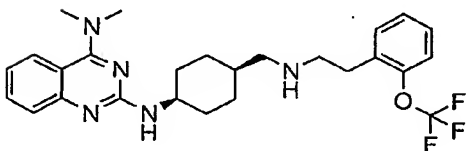
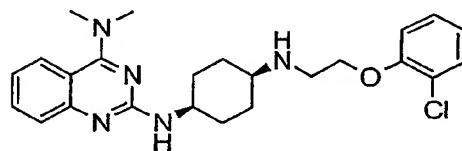
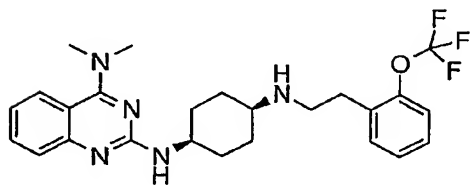
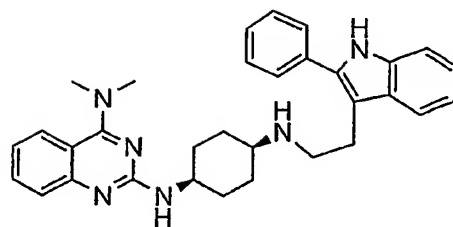
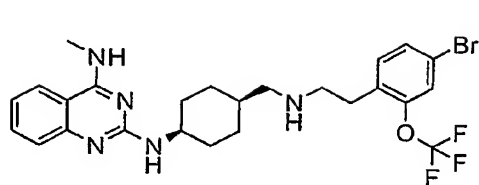
carbocyclyl is acenaphthyl;

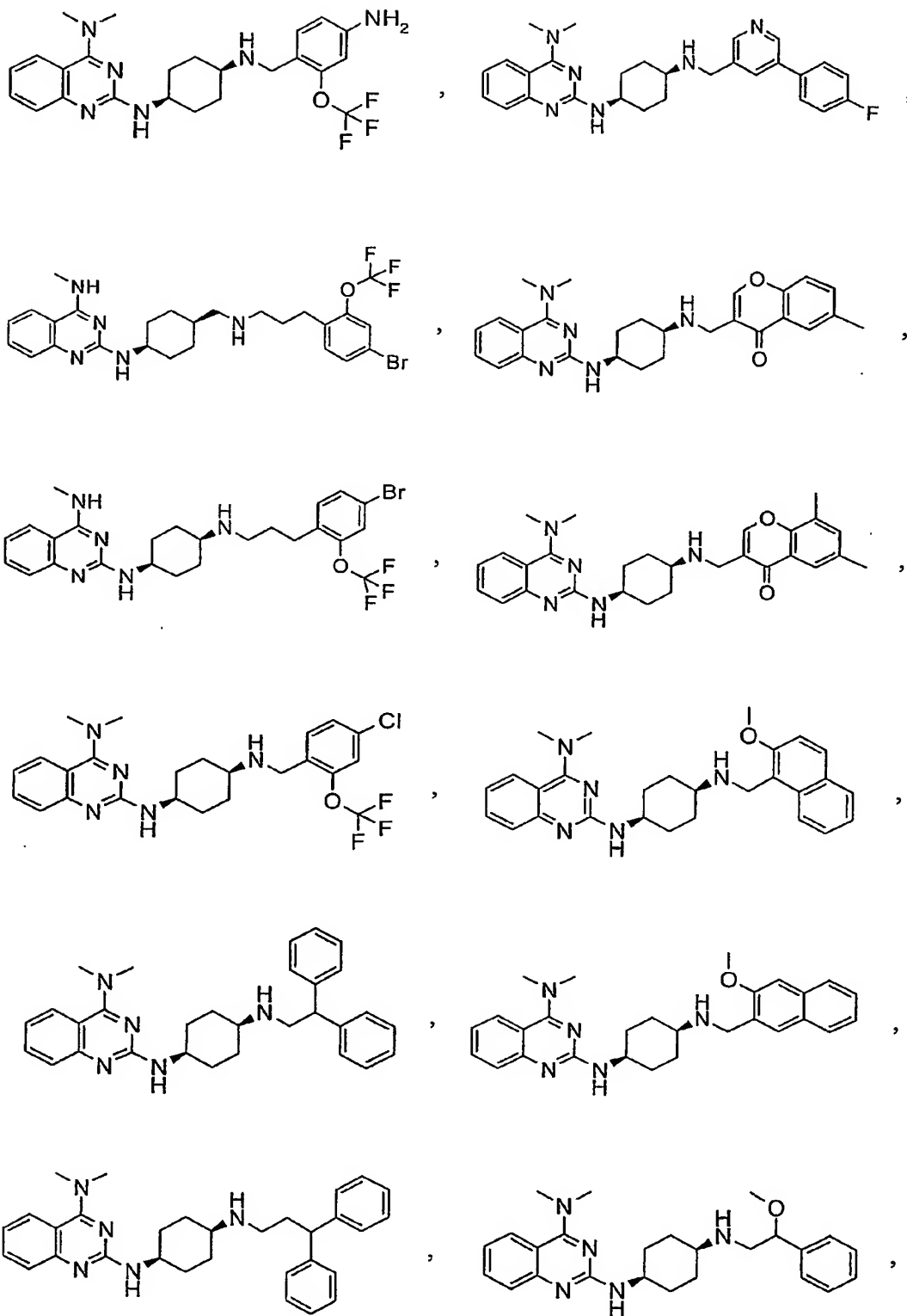
heterocyclyl is 1*H*-indolyl, 1*H*-pyrrolyl, 2,3-dihydro-benzo[1,4]dioxinyl, 9*H*-carbazolyl, benzo[1,3]dioxolyl, furyl, pyrazolyl, thienyl, 4-oxo-benzopyranyl, azetidiny, imidazo[2,1-*b*]thiazolyl, pyridyl, imidazolyl, 2,3-dihydro-benzofuryl, or benzo[*b*]thienyl;
halogen is fluoro, chloro, bromo, or iodo;
or a salt thereof.

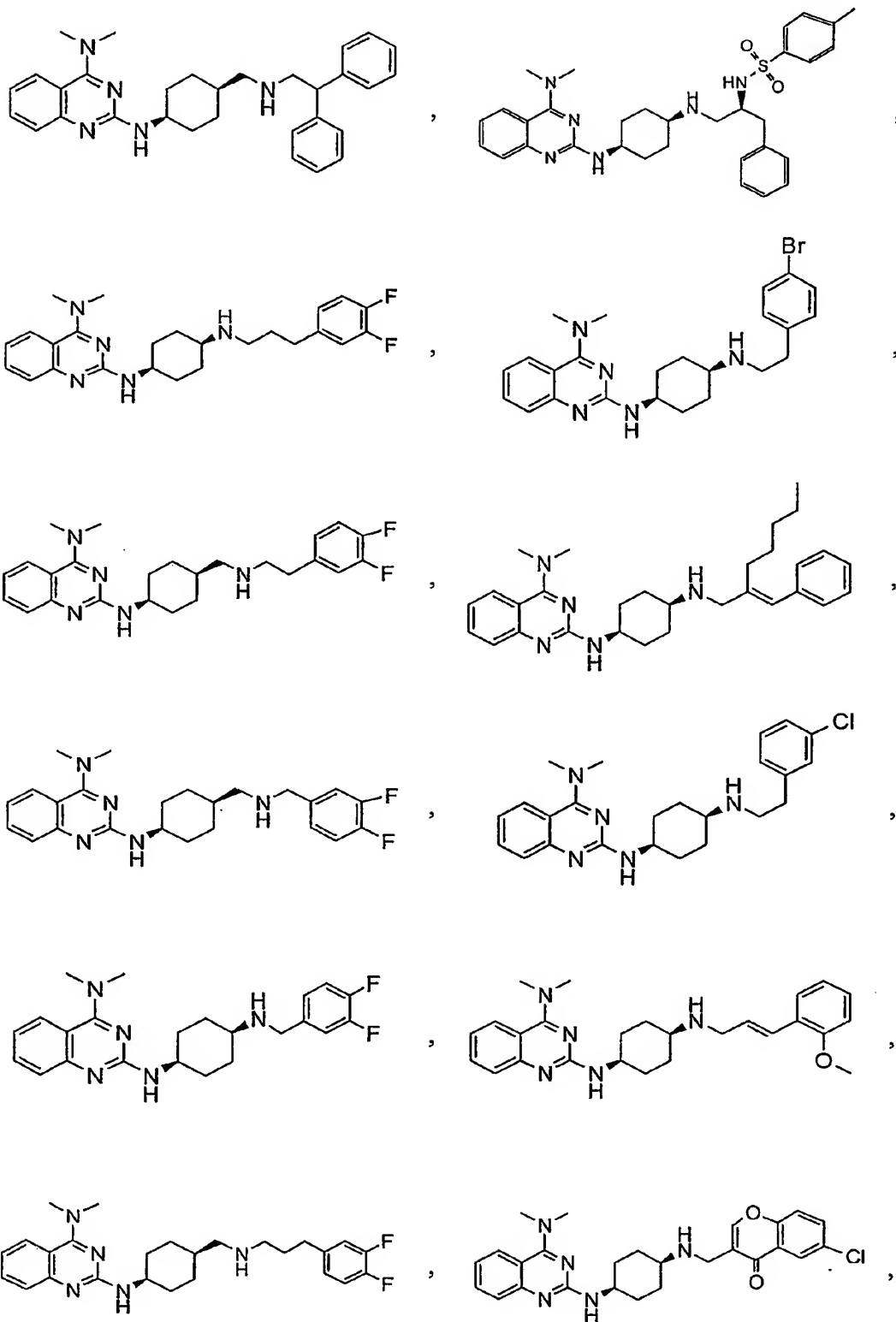
13. A compound according to claim 12 of Formua I selected from the group consisting of

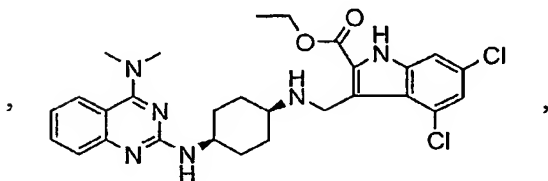
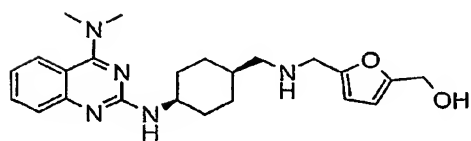
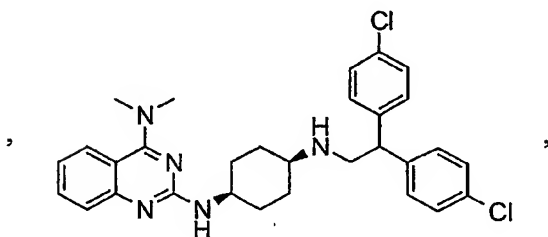
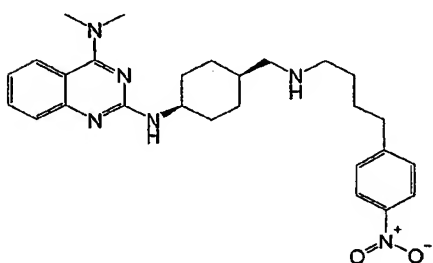
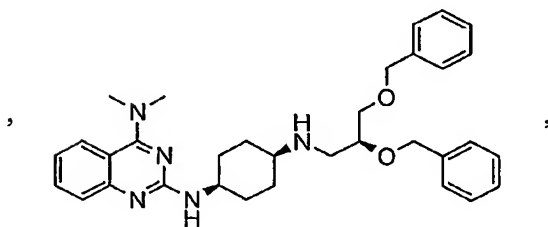
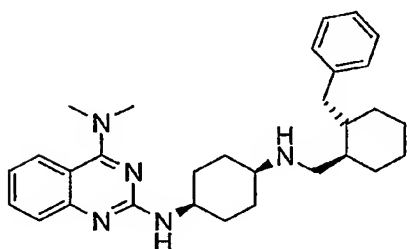
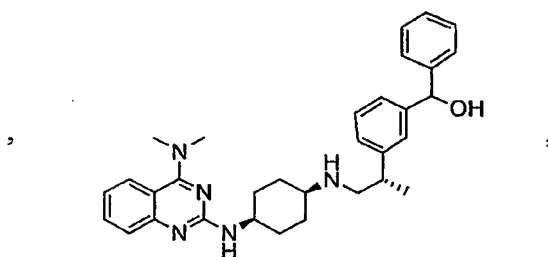
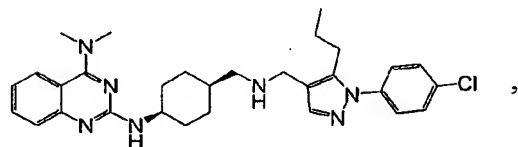
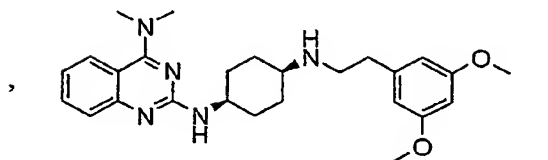
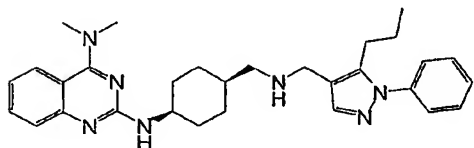
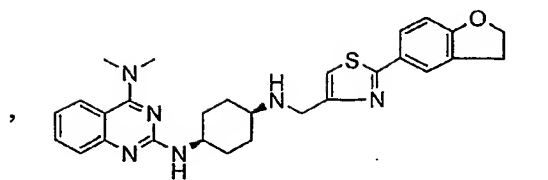
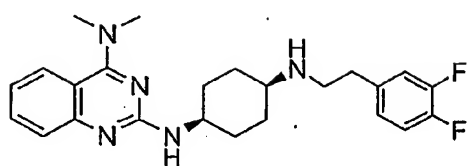


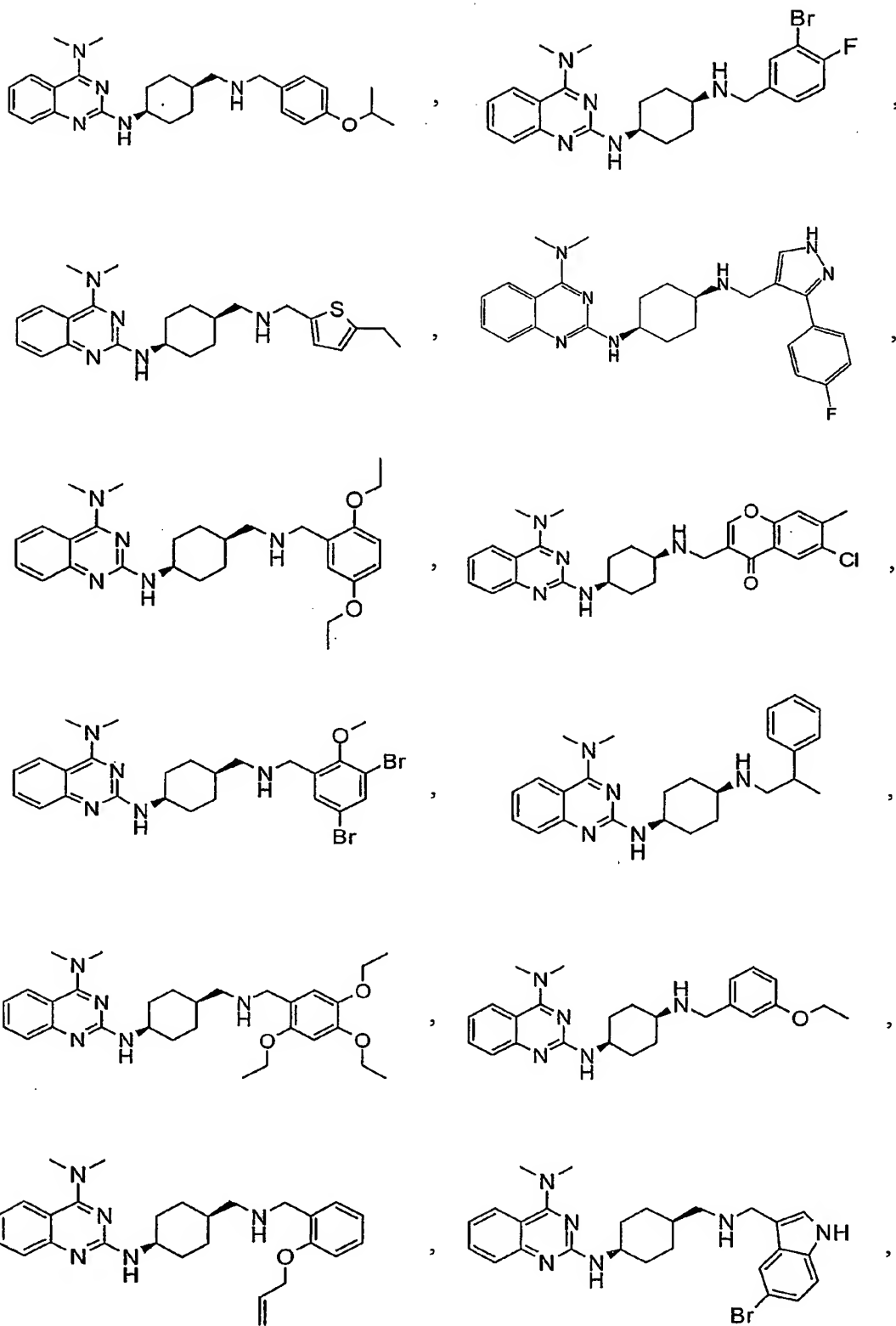


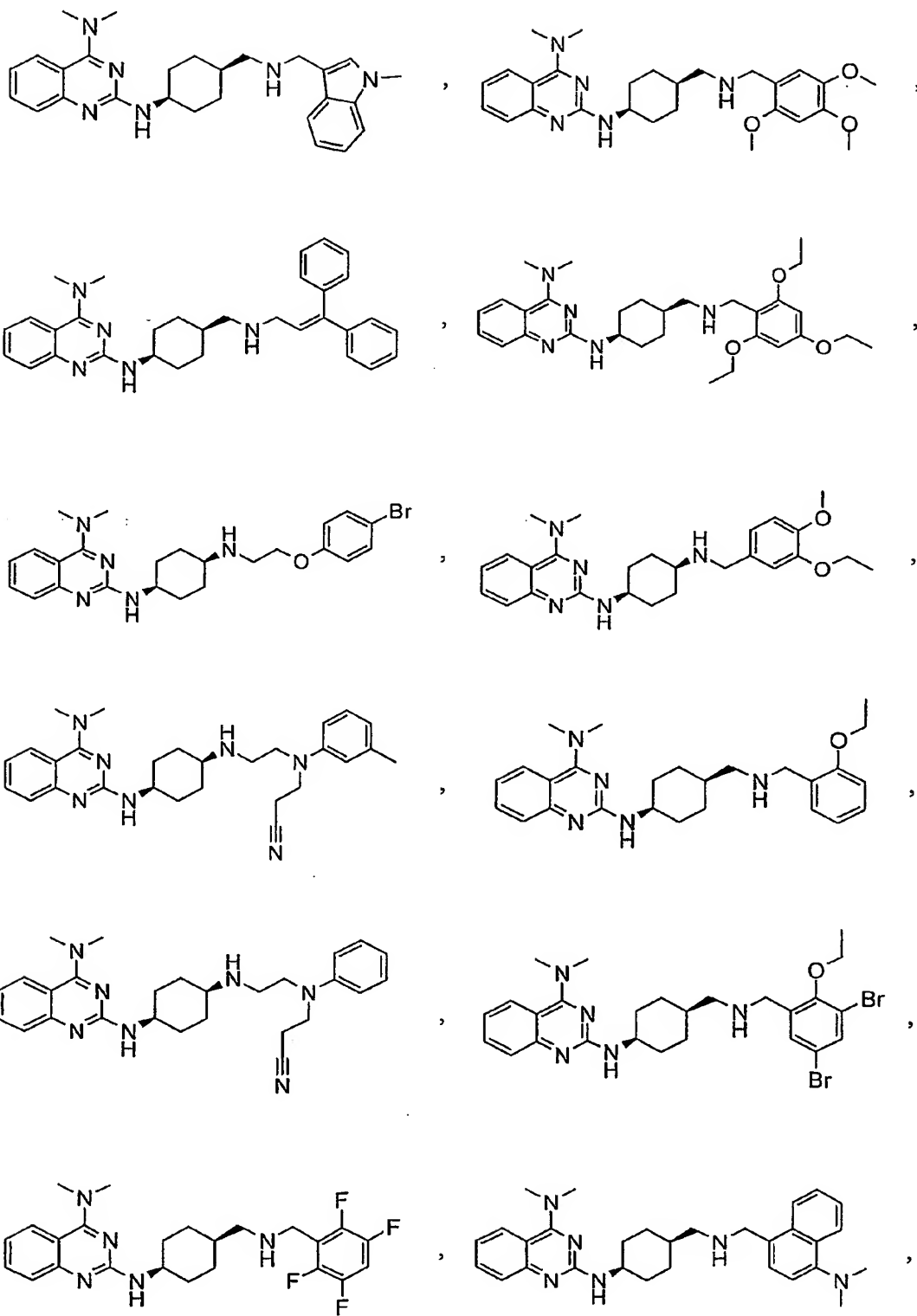


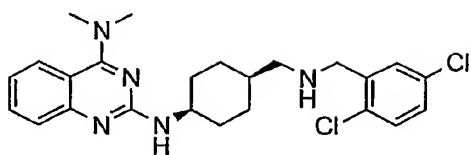




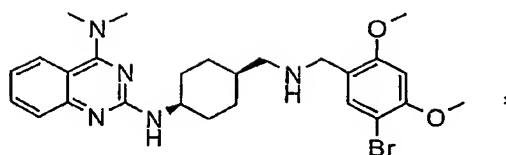




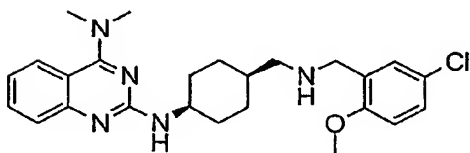




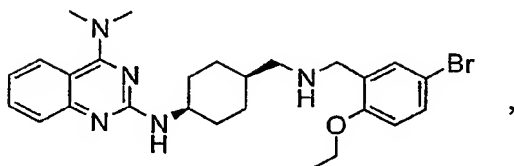
,



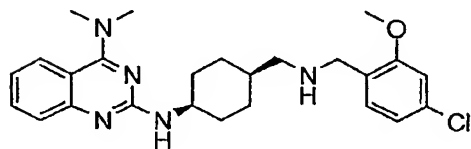
,



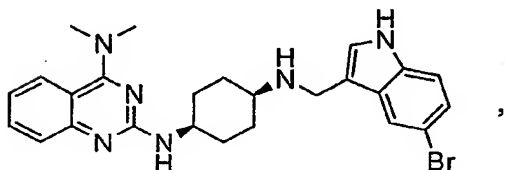
,



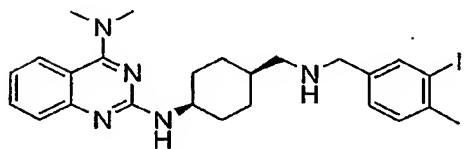
,



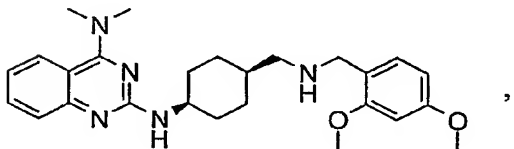
,



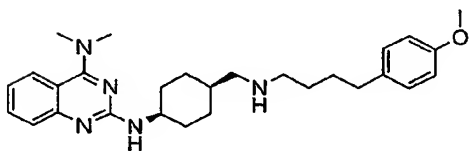
,



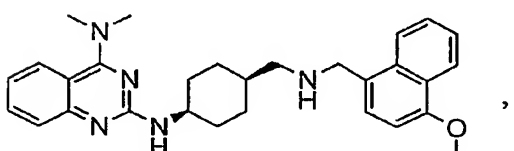
,



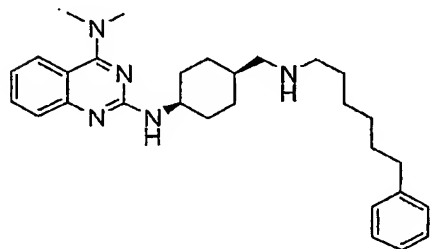
,



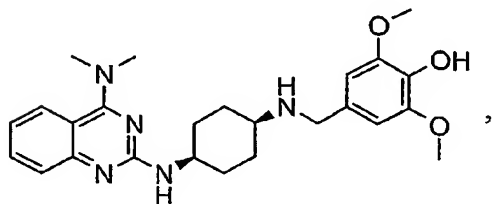
,



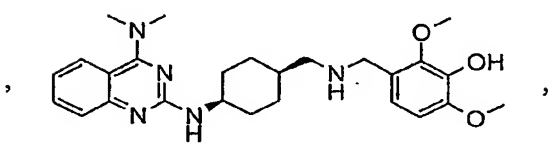
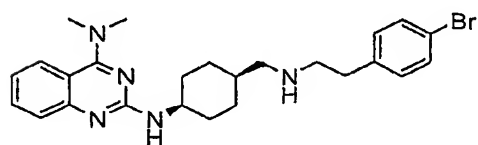
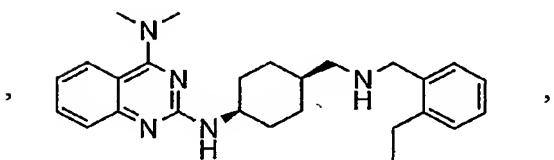
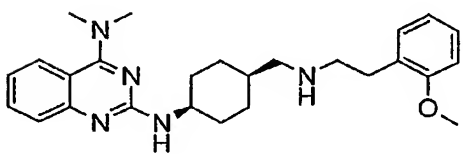
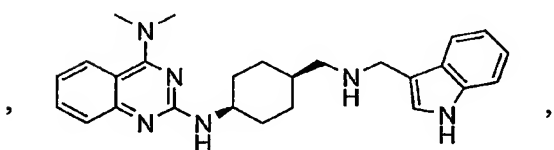
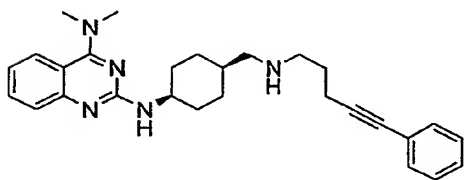
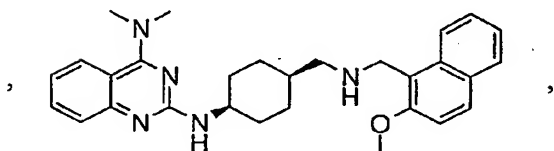
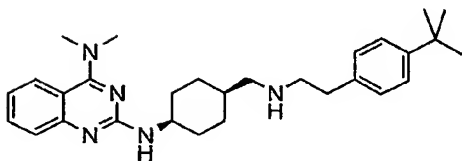
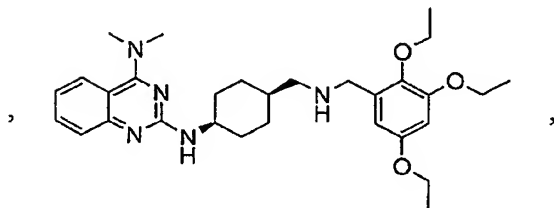
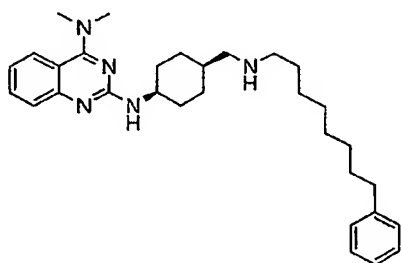
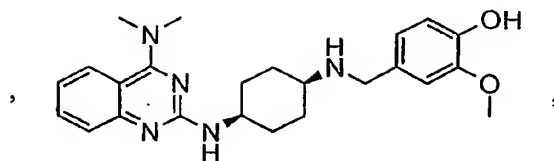
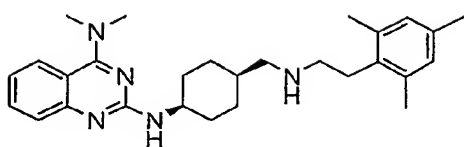
,

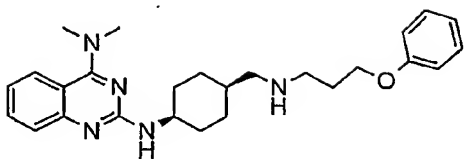


,

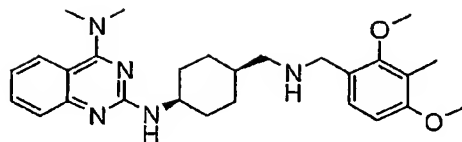


,

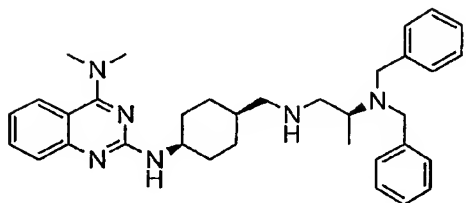




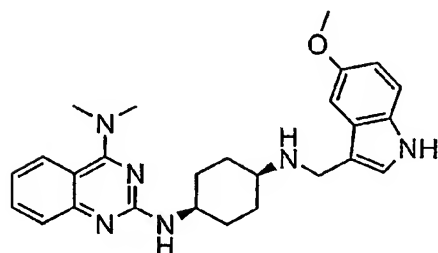
,



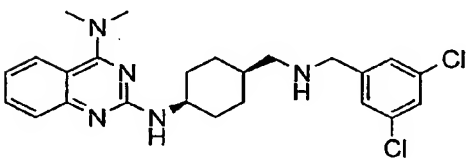
,



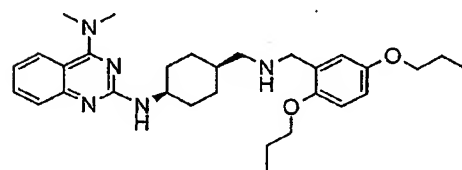
,



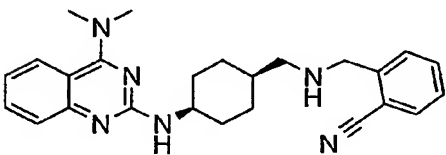
,



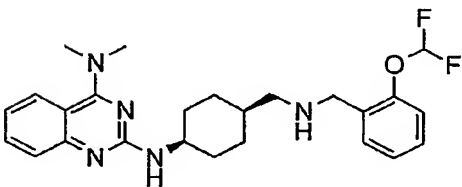
,



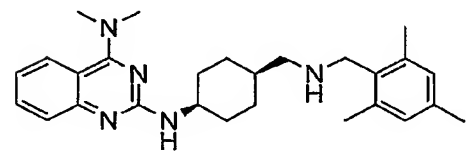
,



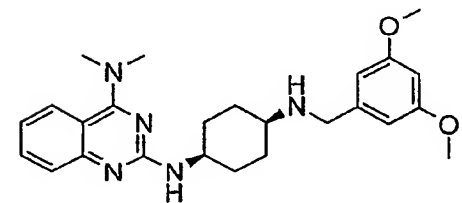
,



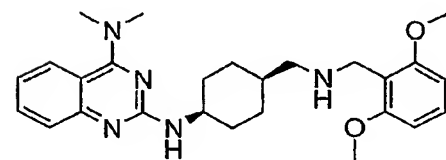
,



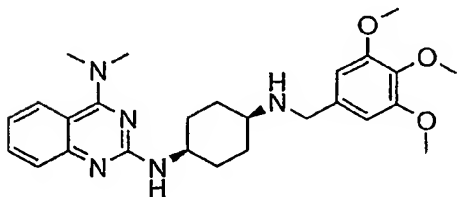
,



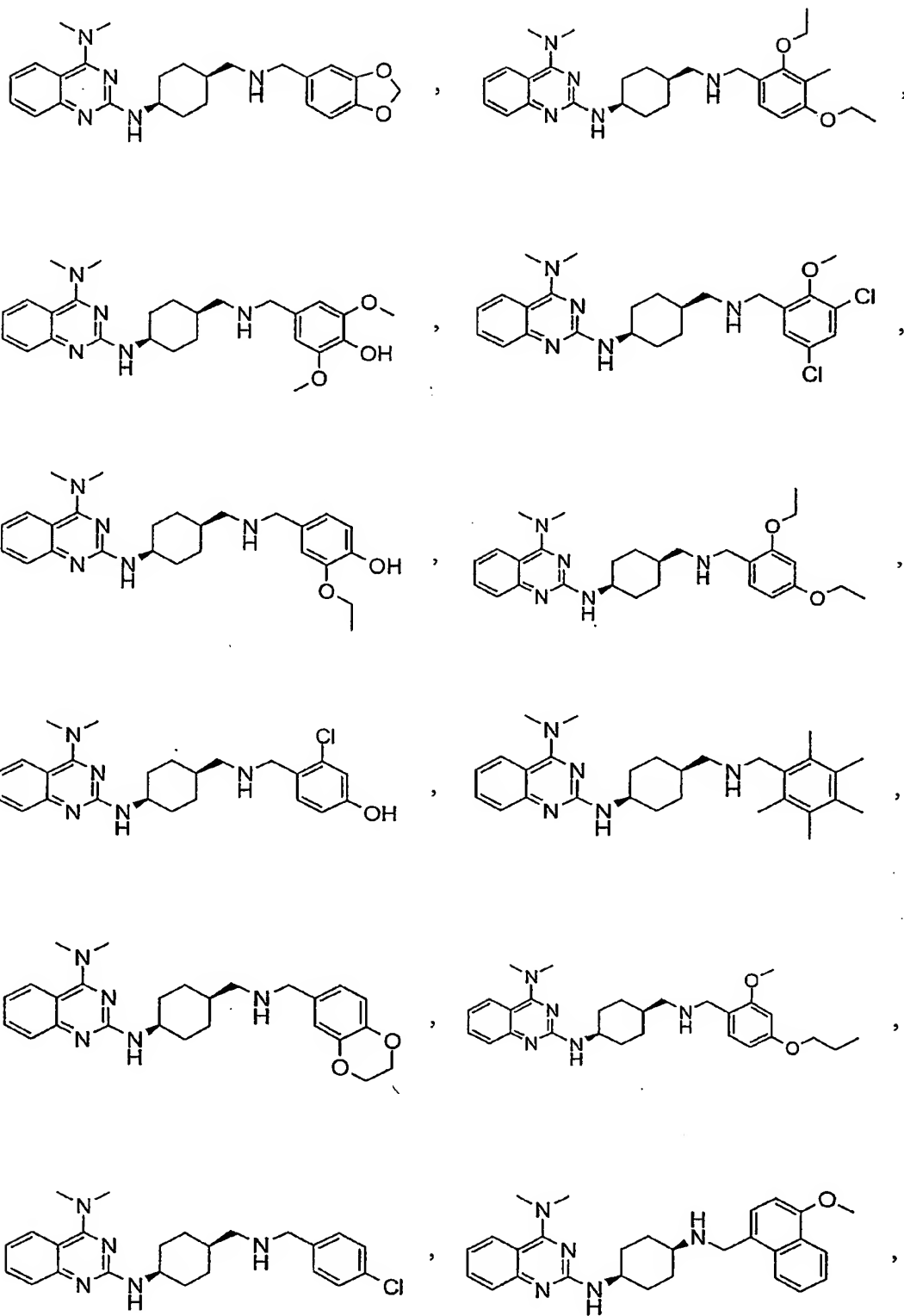
,

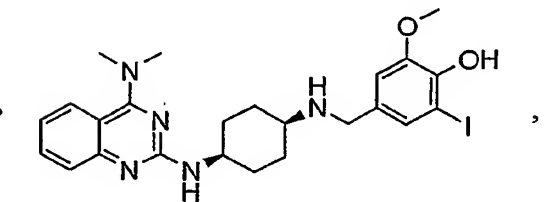
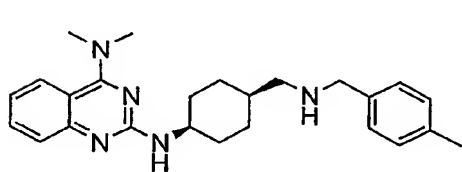
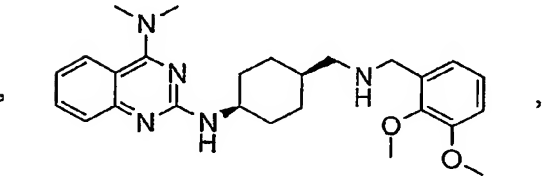
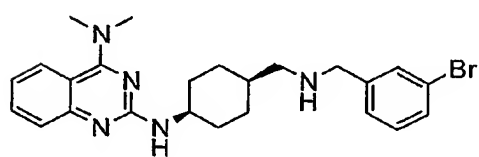
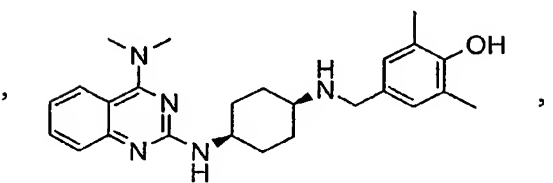
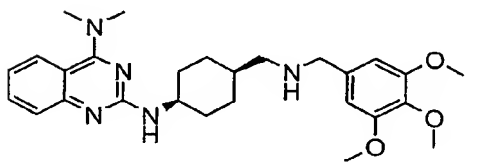
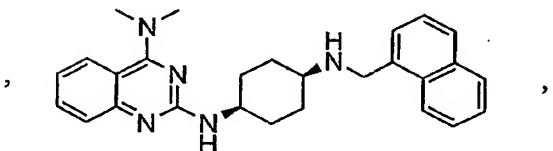
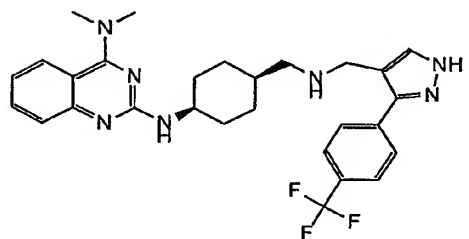
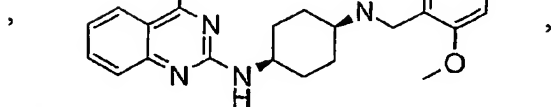
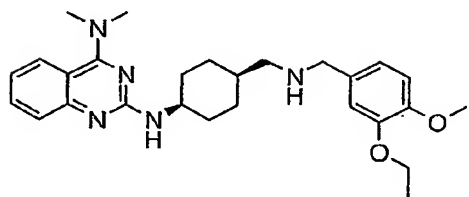
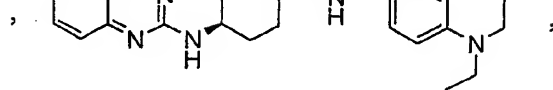
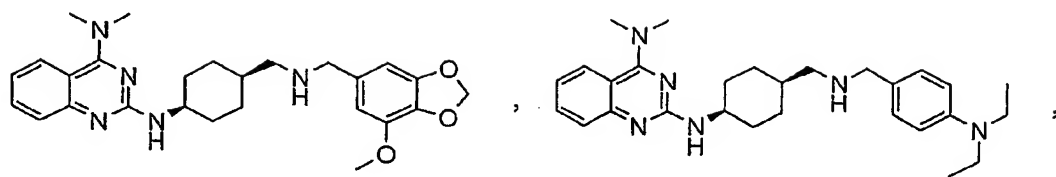


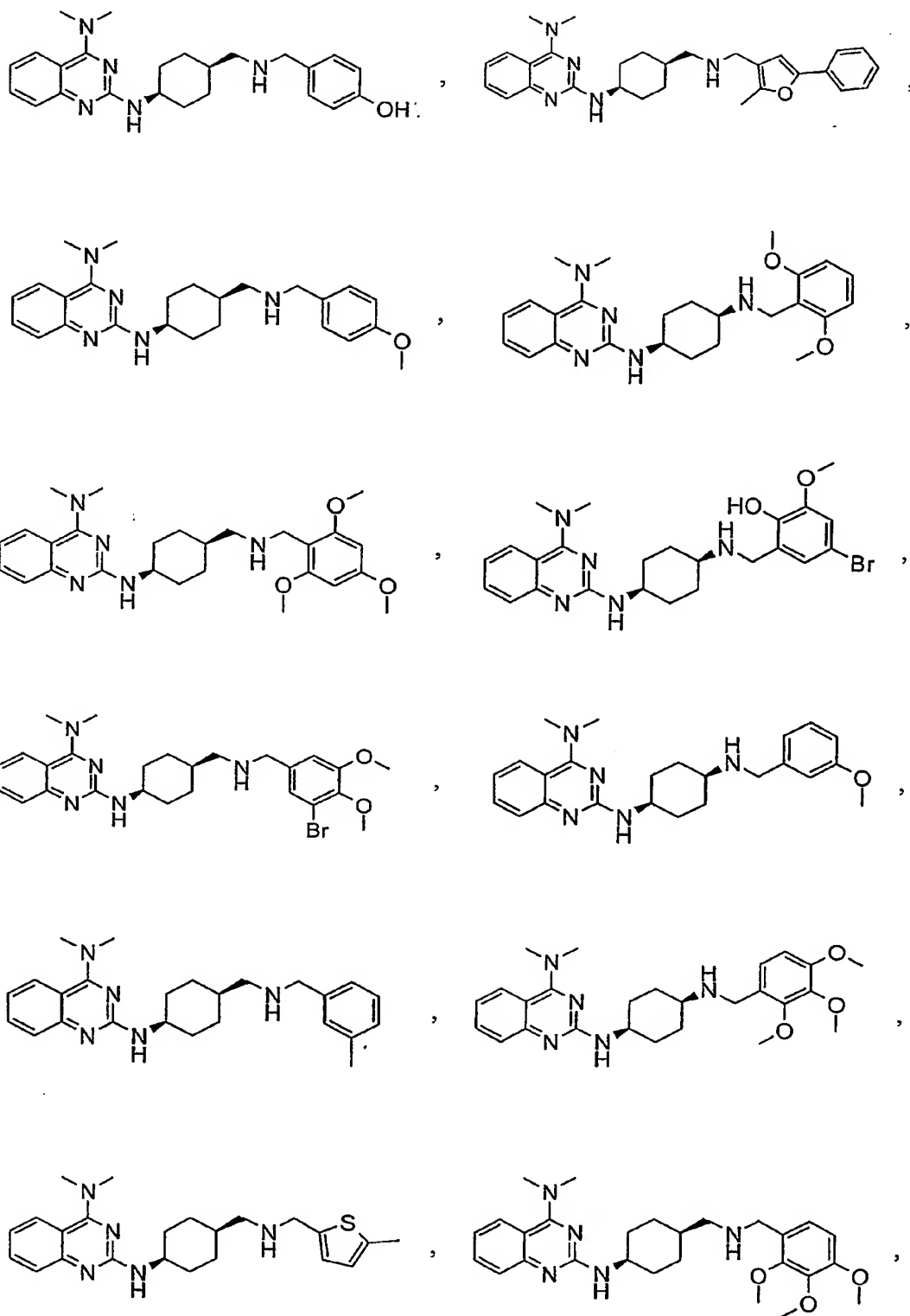
,

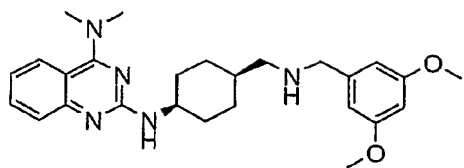


,

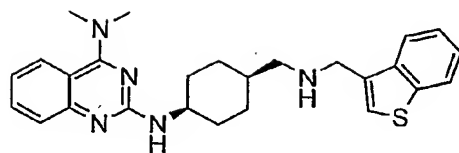




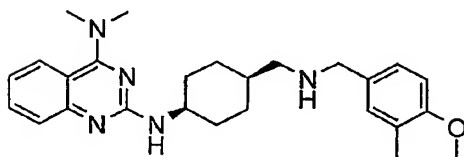




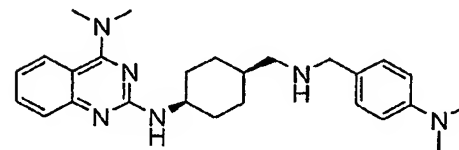
,



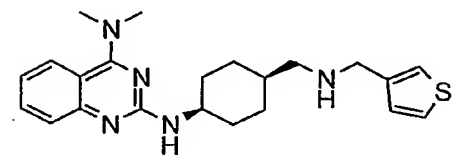
,



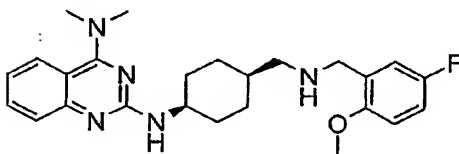
,



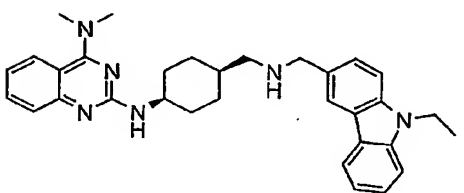
,



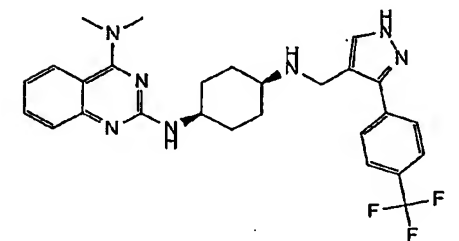
,



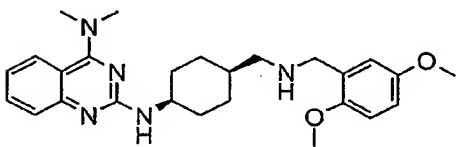
,



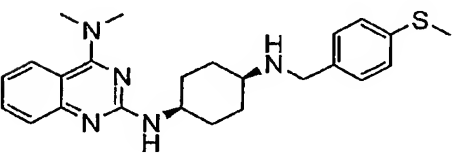
,



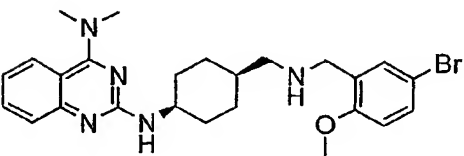
,



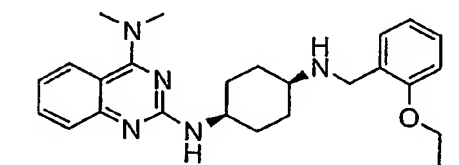
,



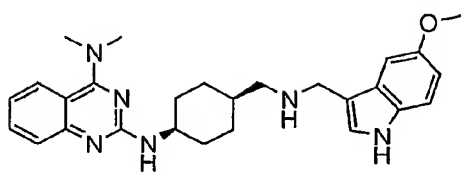
,



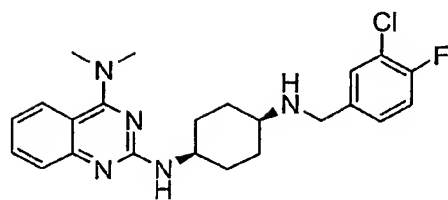
,



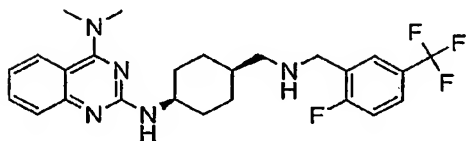
,



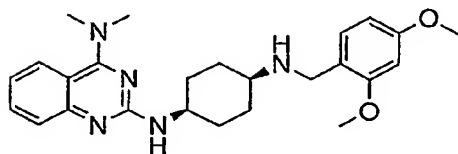
,



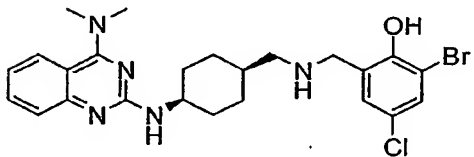
,



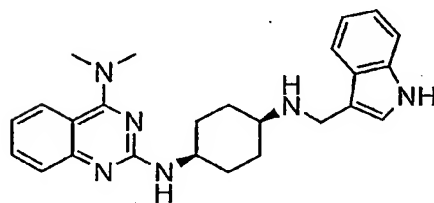
,



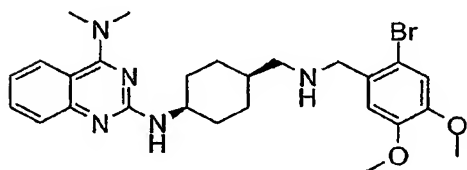
,



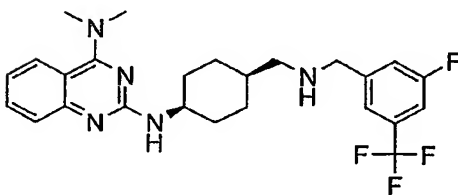
,



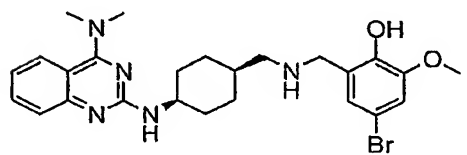
,



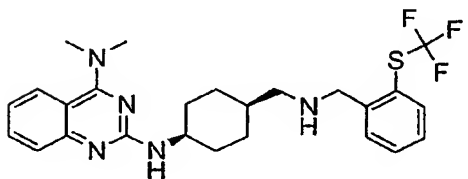
,



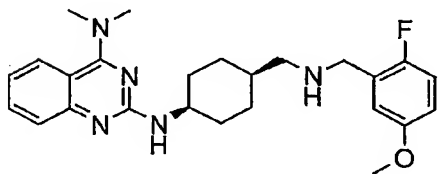
,



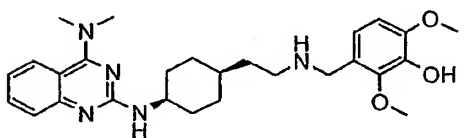
,



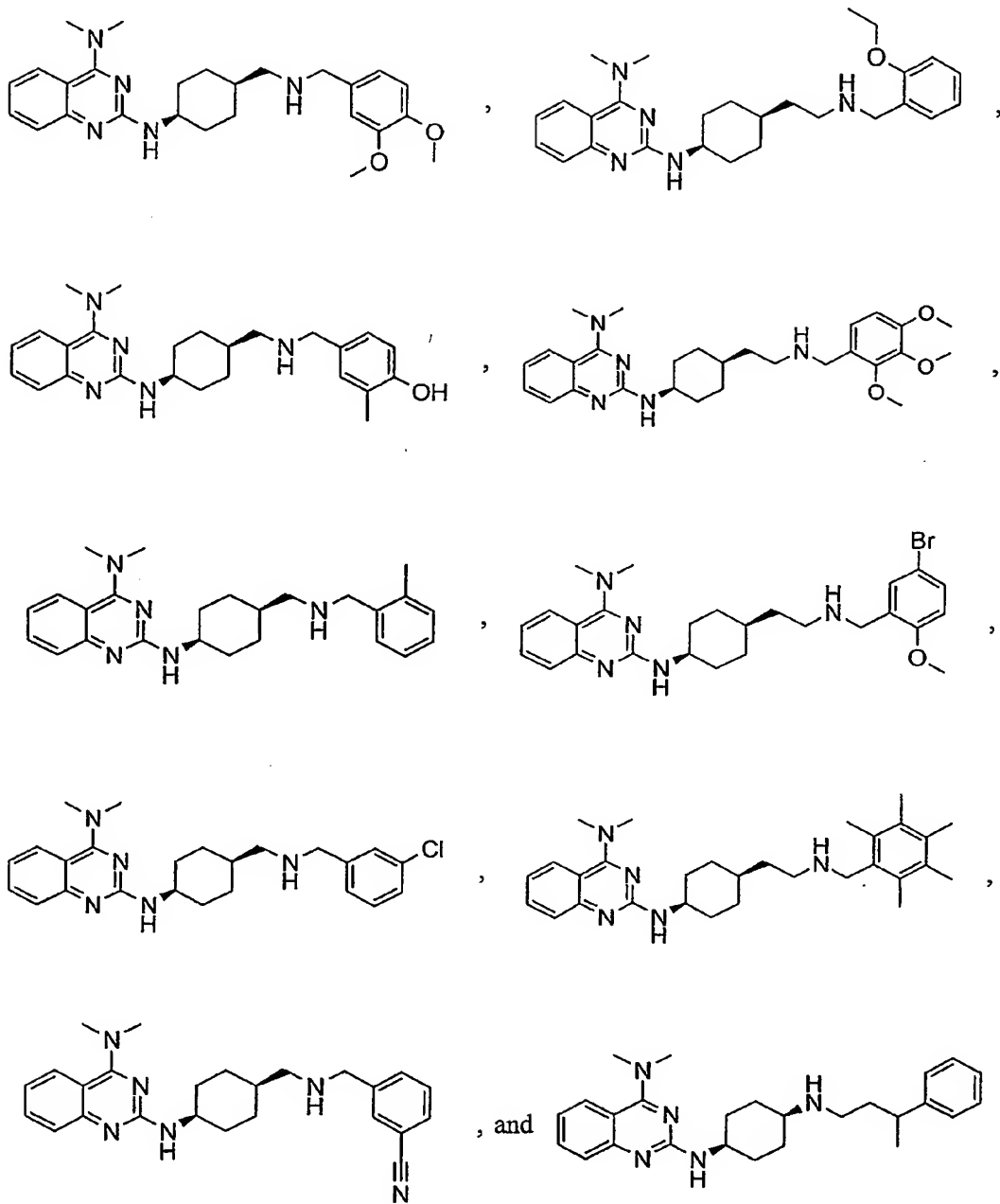
,



,



,



; or, in case of, a salt thereof.

14. A compound according to claim 1, wherein Q is Formula II;

R₁ represents

(i) C₁-C₁₆ alkyl,

C₁-C₁₆ alkyl substituted by substituent(s) independently selected from

•halogen,

•carbocyclyl,

•carbocyclic aryl,

•carbocyclic aryl substituted by substituent(s) independently selected from

••halogen,

••nitro,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

••C₁-C₃ alkoxy,

••halogenated C₁-C₃ alkoxy,

(ii) C₂-C₃ alkenyl,

C₂-C₃ alkenyl substituted by carbocyclic aryl,

(iii) carbocyclic aryl,

carbocyclic aryl substituted by substituent(s) independently selected from

•halogen,

•cyano,

•nitro,

•C₁-C₅ alkyl,

•C₁-C₅ alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

•C₂-C₃ alkenyl,

•C₁-C₄ alkoxy,

•C₁-C₄ alkoxy substituted by substituent(s) independently selected from

••halogen,

••heterocyclyl,

••halogenated heterocyclyl,

•carbocyclic aryloxy,

•carbocyclic aryloxy substituted by substituent(s) independently selected from

••halogen,

••nitro,

•heterocyclyloxy,

•heterocyclyloxy substituted by substituent(s) independently selected from

••halogen,

••C₁-C₃ alkyl,

••halogenated C₁-C₃ alkyl,

•C₁-C₃ alkoxycarbonyl,

•mono- or di-C₁-C₄ alkylamino,

•C₁-C₃ alkylcarbonylamino,

•carbocyclic aryl diazo,

•carbocyclic aryl diazo substituted by mono- or di- C₁-C₃ alkylamino,

•C₁-C₃ alkylsulfonyl,

•carbocyclic aryl,

(iv) heterocyclyl,

or heterocyclyl substituted by substituent(s) independently selected from

•halogen,

•C₁-C₃ alkyl,

•C₁-C₃ alkyl substituted by substituent(s) independently selected from

••halogen,

••oxo,

••carbocyclic arylcarbonylamino,

••halogenated carbocyclic arylcarbonylamino,

••heterocyclyl,

••heterocyclyl substituted by substituent(s) independently selected from

•••halogen,

•••C₁-C₃ alkyl,

•••halogenated C₁-C₃ alkyl,

•C₁-C₃ alkoxy,

•C₁-C₃ alkylcarbonylamino,

•carbocyclic arylsulfonyl,

- C₁-C₃ alkoxy carbonyl,
- carbocyclic aryl,
- halogenated carbocyclic aryl,
- heterocyclyl,
- heterocyclyl substituted by substituent(s) independently selected from
 - halogen,
 - C₁-C₃ alkyl,
 - halogenated C₁-C₃ alkyl;

Y is -S(O)₂-;

wherein carbocyclic aryl is phenyl, biphenyl, or naphthyl;

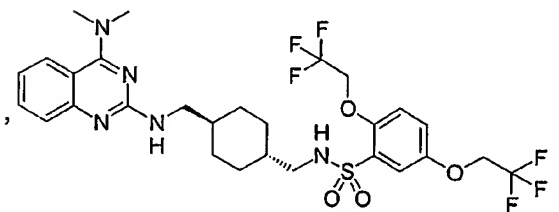
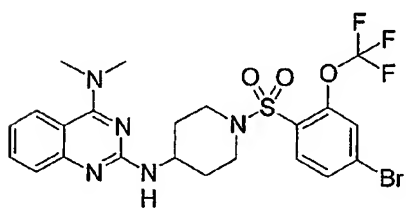
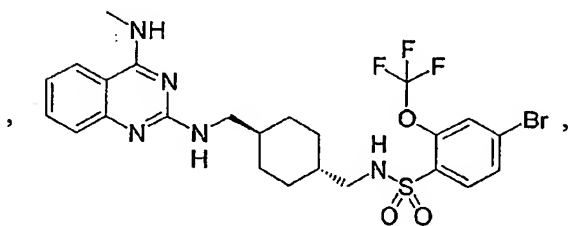
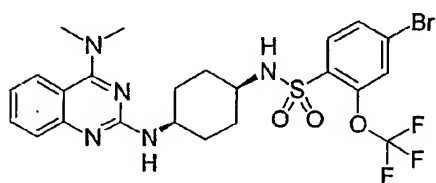
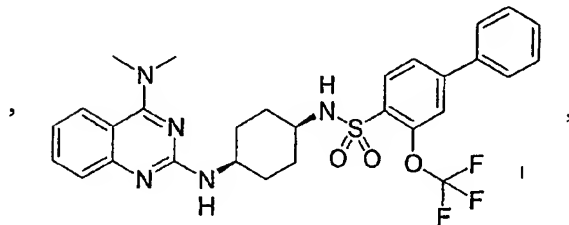
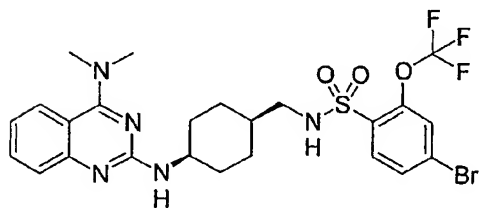
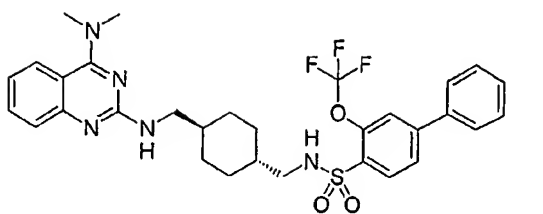
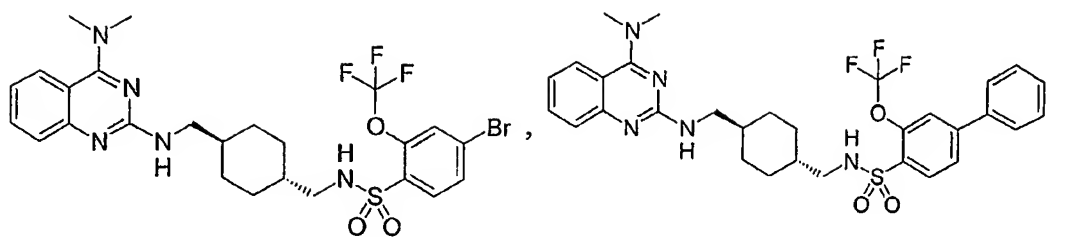
carbocyclyl is 7,7-dimethyl-2-oxo-bicyclo[2.2.1]heptyl;

heterocyclyl is 1,2,3,4-tetrahydro-isoquinolyl, 1,2,3-thiadiazolyl, 1*H*-pyrrolyl, benzo[2,1,3]oxadiazolyl, benzo[b]thienyl, furyl, imidazolyl, isoxazolyl, pyrazolyl, pyridyl, quinolyl, thiazolyl, or thienyl;

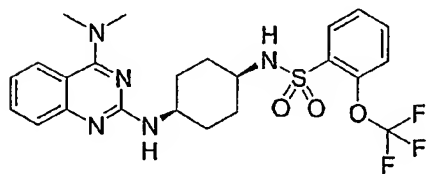
halogen is fluoro, chloro, bromo, or iodo;

or a salt thereof.

15. A compound according to claim 14 of Formua I selected from the group consisting of



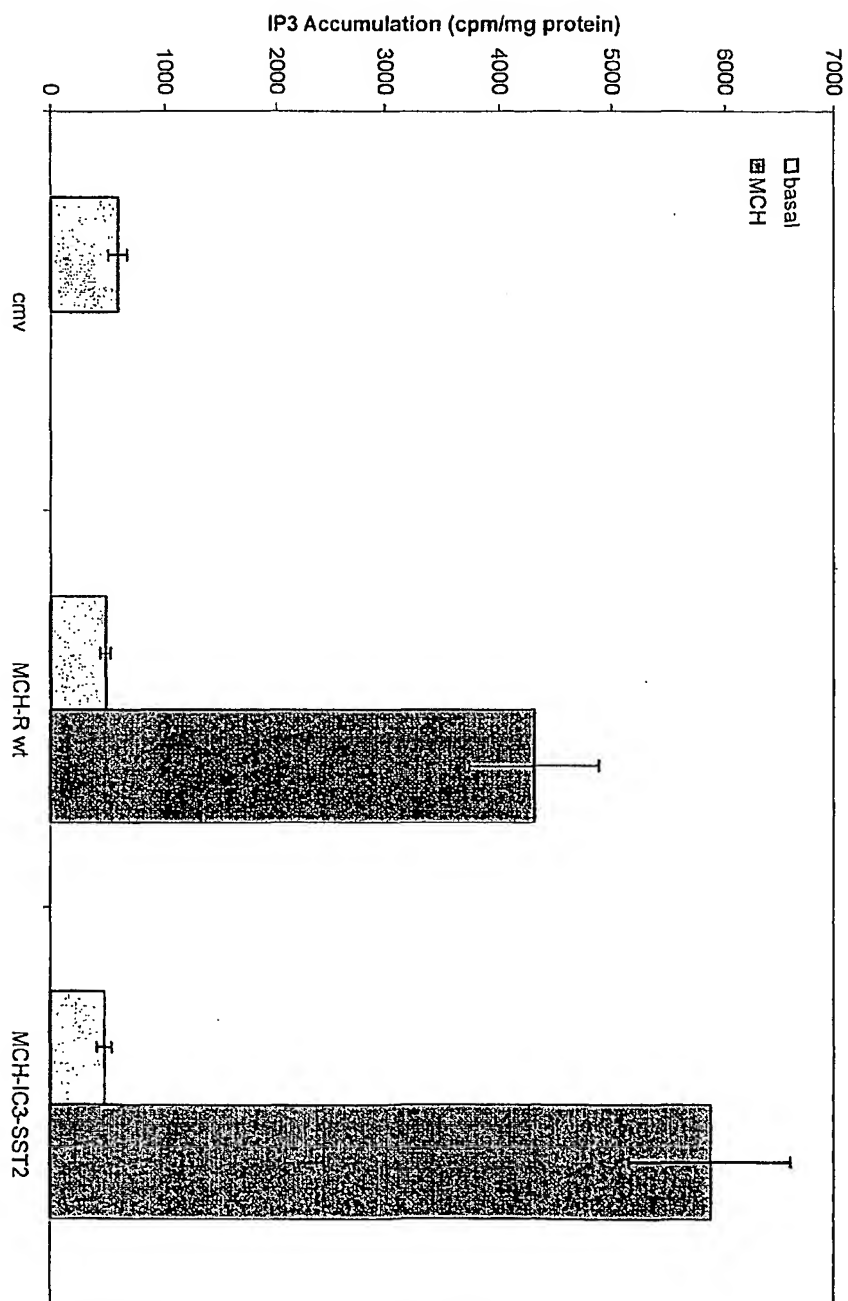
and



; or, in case of, a salt thereof.

16. A compound according to claim 1, wherein Q is Formula II;
R₁ is selected from H, -CO₂^tBu, or -CO₂Bn (Bn is a benzyl group);
R₂ is methylamino or dimethylamino;
L is selected from Formula XX - XXII;
Y is a single bond;
or a salt thereof.
17. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a MCH receptor antagonist.
18. A method for modulating the G-protein receptor, SLC-1, comprising the step of contacting said SLC-1 with a compound of claims 1-16.
19. The method of prophylaxis or treatment of obesity, obesity related disorders, anxiety, or depression in mammals in need of such treatment comprising administering to the mammal a therapeutically effective amount of a compound having the composition of any of claims 1-16.
20. A pharmaceutical composition comprising a pharmaceutically acceptable carrier and a therapeutically effective amount of a compound having the composition of any of claims 1-16.

Fig. 1



SEQUENCE LISTING

<110> Arena Pharmaceuticals, Inc.

<120> MCH Receptor Antagonists

<130> AREN-0238

<160> 12

<170> PatentIn version 3.0

<210> 1

<211> 30

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 1

gtgaagcttg cctctggtgc ctgcaggagg

30

<210> 2

<211> 31

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 2

gcagaattcc cggaggcgtg ttgtggtgcc c

31

<210> 3

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 3

catgagctgg tggatcatga aggg

24

<210> 4

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 4

atgaaggga tgcccaggag aaag

24

<210> 5

<211> 1349

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 5

atggacctgg aagcctcgct gctgccact ggtcccaatg ccagcaacac ctctgatggc 60

cccgataacc tcacttcggc aggatcacct cctcgcacgg ggagcatctc ctacatcaac 120

atcatcatgc cttcgggtgtt cggcaccatc tgcctcctgg gcatcatcgg gaactccacg 180
gtcatcttcg cggtcgtgaa gaagtccaag ctgcactggg gcaacaacgt ccccgacatc 240
ttcatcatca acctctcggg agtagatctc ctctttctcc tgggcatgcc cttcatgac 300
caccagctca tgggcaatgg ggtgtggcac tttggggaga ccatgtgcac cctcatcacg 360
gccatggatg ccaatagtca gttcaccagc acctacatcc tgaccgccat ggccattgac 420
cgctacctgg ccactgtcca ccccatctct tccacgaagt tccggaagcc ctctgtggcc 480
accctgggta tctgcctcct gtggggccctc tccttcatca gcatcaccoc tgtgtggctg 540
tatgccagac tcatccctt cccaggagggt gcagtgggct gcggcatacg cctgcccac 600
ccagacactg acctctactg gttcacctg taccagtttt tctggcctt tgccctgcct 660
tttgtggtea tcacagccgc atacgtgagg atcctgcaga aggtgaagtc ctctggaatc 720
cgagtgggct cctctaagag gaagaagtct gagaagaagg tcacccgcac agccatcgcc 780
atctgtctgg tcttctttgt gtgctgggca ccctactatg tgctacagct gaccagttg 840
tccatcagcc gcccgacct cacctttgtc tacttataca atgcggccat cagcttgggc 900
tatgccaaca gctgcctcaa cccctttgtg tacatcgtgc tctgtgagac gttccgcaaa 960
cgcttggtec tgtcggtgaa gcctgcagcc caggggcagc ttgcgctgt cagcaacgct 1020
cagacggctg acgaggagag gacagaaagc aaaggcacct gatacttccc ctgccaccct 1080
gcacacctcc aagtcagggc accacaacac gccaccggga gagatgctga gaaaaacca 1140
agaccgctcg ggaaatgcag gaaggccggg ttgtgagggg ttgttgcaat gaaataaata 1200
cattccatgg gctcacacgt tgctggggag gcctggagtc aggtttgggg ttttcagata 1260
tcagaaatcc cttgggggag caggatgaga cctttggata gaacagaagc tgagcaagag 1320
aacatgttgg tttggataac cggttgcac 1349

<210> 6

<211> 446

<212> PRT

<213> Homo Sapien

<220>

<223> Novel Sequence

<400> 6

```

Met Asp Leu Glu Ala Ser Leu Leu Pro Thr Gly Pro Asn Ala Ser Asn
 1           5           10           15

Thr Ser Asp Gly Pro Asp Asn Leu Thr Ser Ala Gly Ser Pro Pro Arg
 20           25           30

Thr Gly Ser Ile Ser Tyr Ile Asn Ile Ile Met Pro Ser Val Phe Gly
 35           40           45

Thr Ile Cys Leu Leu Gly Ile Ile Gly Asn Ser Thr Val Ile Phe Ala
 50           55           60

Val Val Lys Lys Ser Lys Leu His Trp Cys Asn Asn Val Pro Asp Ile
 65           70           75           80

Phe Ile Ile Asn Leu Ser Val Val Asp Leu Leu Phe Leu Leu Gly Met
           85           90           95

Pro Phe Met Ile His Gln Leu Met Gly Asn Gly Val Trp His Phe Gly
           100           105           110

Glu Thr Met Cys Thr Leu Ile Thr Ala Met Asp Ala Asn Ser Gln Phe
           115           120           125

Thr Ser Thr Tyr Ile Leu Thr Ala Met Ala Ile Asp Arg Tyr Leu Ala
           130           135           140

Thr Val His Pro Ile Ser Ser Thr Lys Phe Arg Lys Pro Ser Val Ala
           145           150           155           160

Thr Leu Val Ile Cys Leu Leu Trp Ala Leu Ser Phe Ile Ser Ile Thr
           165           170           175

Pro Val Trp Leu Tyr Ala Arg Leu Ile Pro Phe Pro Gly Gly Ala Val
           180           185           190

Gly Cys Gly Ile Arg Leu Pro Asn Pro Asp Thr Asp Leu Tyr Trp Phe
           195           200           205

Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
           210           215           220

Thr Ala Ala Tyr Val Arg Ile Leu Gln Lys Val Lys Ser Ser Gly Ile
           225           230           235           240

Arg Val Gly Ser Ser Lys Arg Lys Lys Ser Glu Lys Lys Val Thr Arg
           245           250           255

Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
           260           265           270

Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
           275           280           285

Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser

```

290 295 300
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys
 305 310 315 320
 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala
 325 330 335
 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly
 340 345 350
 Thr Tyr Phe Pro Cys His Pro Ala His Leu Gln Val Arg Ala Pro Gln
 355 360 365
 His Ala Thr Gly Arg Asp Ala Glu Lys Asn Pro Arg Pro Leu Gly Lys
 370 375 380
 Cys Arg Lys Ala Gly Leu Gly Val Val Ala Met Lys Ile His Ser Met
 385 390 395 400
 Gly Ser His Val Ala Gly Glu Ala Trp Ser Gln Val Trp Gly Phe Gln
 405 410 415
 Ile Ser Glu Ile Pro Trp Gly Ser Arg Met Arg Pro Leu Asp Arg Thr
 420 425 430
 Glu Ala Glu Gln Glu Asn Met Leu Val Trp Ile Thr Gly Cys
 435 440 445

<210> 7
 <211> 70

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 7
 gatcctgcag aaggtgaagt cctctggaat ccgagtgggc tcctctaaga ggaagaagtc 60
 tgagaagaag 70

<210> 8

<211> 71

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 8

gtgaccttct tctcagactt ctctctctta gaggagccca ctcgattcc agaggacttc 60

accttctgca g 71

<210> 9

<211> 30

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 9

gtgaagcttg cccgggcagg atggacctgg 30

<210> 10

<211> 24

<212> DNA

<213> Artificial

<220>

<223> Novel Sequence

<400> 10

atctagaggt gcctttgctt tctg 24

<210> 11

<211> 2133

<212> DNA

<213> Homo Sapien

<400> 11

atggacctgg aagcctcgct gctgccact ggtccaatg ccagcaaac ctctgatggc 60

cccgataacc tcacttcggc aggatcacct cctcgcacgg ggagcatctc ctacatcaac 120

atcatcatgc cttcggtgtt cggcaccatc tgcctcctgg gcatcatcgg gaactccacg 180
gtcatcttcg cggctcgtgaa gaagtcacag ctgcactggt gcaacaacgt ccccgacatc 240
ttcatcatca acctctcggg agtagatctc ctctttctcc tgggcatgcc ctcatgatc 300
caccagctca tgggcaatgg ggtgtggcac tttggggaga ccatgtgcac cctcatcacg 360
gccatggatg ccaatagtca gttcaccagc acctacatcc tgaccgcat ggccattgac 420
cgctacctgg ccaactgtcca ccccatctct tccacgaagt tccggaagcc ctctgtggcc 480
accctggtga tctgcctcct gtgggccctc tccttcacga gcatcacccc tgtgtggctg 540
tatgccagac tcacccctt cccaggaggt gcagtgggt gcggcatacg cctgcccaac 600
ccagacactg acctctactg gttcacctg taccagttt tcctggcctt tgccctgcct 660
tttgtggtca tcacagccgc atacgtgagg atcctgcagc gcatgacgtc ctacgtggcc 720
cccgctccc agcgcagcat cgggtgcgg acaaagagg tgaccgcac agccatcgcc 780
atctgtctgg tcttcttctgt gtgtgggca ccctactatg tgctacagct gaccagttg 840
tccatcagcc gcccgacct cacctttgtc tacttataca atgcggccat cagcttgggc 900
tatgccaaac gctgcctcaa cccctttgtg tacatcgtgc tctgtgagac gttccgcaa 960
cgcttggtcc tgcggtgaa gcctgcagcc caggggcagc ttcgctgtg cagcaacgct 1020
cagacggctg acgaggagag gacagaaagc aaaggcacct ctagaatggg ctgcacactg 1080
agcgtgagg acaaggcggc cgtggagcgc agcaagatga tcgaccgcaa cctccgggag 1140
gacggagaga aggcagcgc cgaggtcaag ctgctgtgc tgggtgctg tgaatccggg 1200
aagagcaca ttgtgaagca gatgaaaatt atccacgagg ctggctactc agaggaagag 1260
tgtaagcagt acaaagcagt ggtctacagc aacaccatcc agtccatcat tgccatcatt 1320
agagccatgg ggagattgaa aatcgacttt ggagacgctg ctgctgcgga tgatgctcgc 1380
caactcttcg tgcttgctgg ggctgcagag gaaggcttta tgaccgcgga gctcgccggc 1440
gtcataaaga gactgtgaa ggacagcggg gtgcaagcct gcttcaacag atcccgggag 1500
taccagctga acgattcggc ggcgtactac ctgaatgact tggacagaat agcacaacca 1560
aattacatcc caaccagca ggatgttctc agaactagag tgaaaacgac gggaattgtg 1620
gaaaccact ttactttcaa agatcttcat tttaaaatgt ttgacgtggg aggcagaga 1680
tcagagcgga agaagtggat tcaactgttt gaaggcgtga ctgccatcat cttctgtgtg 1740
gccctgagt actatgacct ggttcttgcg gaggatgaag aaatgaaccg gatgcatgaa 1800
agcatgaagc tgttcgatag catatgtaac aacaagtggg ttacggacac atccatcatc 1860

cttttcctga acaagaagga cctcttcgaa gagaagatca aaaagagtcc cctcacgata 1920
 tgctatccag aatatgcagg ctcaaacaca tatgaagagg cggctgcgta tatccagtgt 1980
 cagtttgaag acctcaataa aaggaaggac acaaaggaaa ttacaccca cttcacttgc 2040
 gccacggata cgaagaatgt gcagtttgtg ttcgatgctg taacggacgt catcataaag 2100
 aataacctaa aagactgtgg tctcttctaa tct 2133

<210> 12

<211> 709

<212> PRT

<213> Homo Sapien

<400> 12

Met	Asp	Leu	Glu	Ala	Ser	Leu	Leu	Pro	Thr	Gly	Pro	Asn	Ala	Ser	Asn
1				5					10					15	
Thr	Ser	Asp	Gly	Pro	Asp	Asn	Leu	Thr	Ser	Ala	Gly	Ser	Pro	Pro	Arg
			20					25					30		
Thr	Gly	Ser	Ile	Ser	Tyr	Ile	Asn	Ile	Ile	Met	Pro	Ser	Val	Phe	Gly
		35					40					45			
Thr	Ile	Cys	Leu	Leu	Gly	Ile	Ile	Gly	Asn	Ser	Thr	Val	Ile	Phe	Ala
	50					55					60				
Val	Val	Lys	Lys	Ser	Lys	Leu	His	Trp	Cys	Asn	Asn	Val	Pro	Asp	Ile
	65				70					75					80
Phe	Ile	Ile	Asn	Leu	Ser	Val	Val	Asp	Leu	Leu	Phe	Leu	Leu	Gly	Met
			85						90					95	
Pro	Phe	Met	Ile	His	Gln	Leu	Met	Gly	Asn	Gly	Val	Trp	His	Phe	Gly
		100						105					110		
Glu	Thr	Met	Cys	Thr	Leu	Ile	Thr	Ala	Met	Asp	Ala	Asn	Ser	Gln	Phe
	115						120					125			
Thr	Ser	Thr	Tyr	Ile	Leu	Thr	Ala	Met	Ala	Ile	Asp	Arg	Tyr	Leu	Ala
	130					135					140				
Thr	Val	His	Pro	Ile	Ser	Ser	Thr	Lys	Phe	Arg	Lys	Pro	Ser	Val	Ala
	145				150				155						160
Thr	Leu	Val	Ile	Cys	Leu	Leu	Trp	Ala	Leu	Ser	Phe	Ile	Ser	Ile	Thr
			165					170					175		
Pro	Val	Trp	Leu	Tyr	Ala	Arg	Leu	Ile	Pro	Phe	Pro	Gly	Gly	Ala	Val
		180					185						190		
Gly	Cys	Gly	Ile	Arg	Leu	Pro	Asn	Pro	Asp	Thr	Asp	Leu	Tyr	Trp	Phe
	195					200						205			

Thr Leu Tyr Gln Phe Phe Leu Ala Phe Ala Leu Pro Phe Val Val Ile
 210 215 220
 Thr Ala Ala Tyr Val Arg Ile Leu Gln Arg Met Thr Ser Ser Val Ala
 225 230 235 240
 Pro Ala Ser Gln Arg Ser Ile Arg Leu Arg Thr Lys Arg Val Thr Arg
 245 250 255
 Thr Ala Ile Ala Ile Cys Leu Val Phe Phe Val Cys Trp Ala Pro Tyr
 260 265 270
 Tyr Val Leu Gln Leu Thr Gln Leu Ser Ile Ser Arg Pro Thr Leu Thr
 275 280 285
 Phe Val Tyr Leu Tyr Asn Ala Ala Ile Ser Leu Gly Tyr Ala Asn Ser
 290 295 300
 Cys Leu Asn Pro Phe Val Tyr Ile Val Leu Cys Glu Thr Phe Arg Lys
 305 310 315 320
 Arg Leu Val Leu Ser Val Lys Pro Ala Ala Gln Gly Gln Leu Arg Ala
 325 330 335
 Val Ser Asn Ala Gln Thr Ala Asp Glu Glu Arg Thr Glu Ser Lys Gly
 340 345 350
 Thr Ser Arg Met Gly Cys Thr Leu Ser Ala Glu Asp Lys Ala Ala Val
 355 360 365
 Glu Arg Ser Lys Met Ile Asp Arg Asn Leu Arg Glu Asp Gly Glu Lys
 370 375 380
 Ala Ala Arg Glu Val Lys Leu Leu Leu Leu Gly Ala Gly Glu Ser Gly
 385 390 395 400
 Lys Ser Thr Ile Val Lys Gln Met Lys Ile Ile His Glu Ala Gly Tyr
 405 410 415
 Ser Glu Glu Glu Cys Lys Gln Tyr Lys Ala Val Val Tyr Ser Asn Thr
 420 425 430
 Ile Gln Ser Ile Ile Ala Ile Ile Arg Ala Met Gly Arg Leu Lys Ile
 435 440 445
 Asp Phe Gly Asp Ala Ala Arg Ala Asp Asp Ala Arg Gln Leu Phe Val
 450 455 460
 Leu Ala Gly Ala Ala Glu Glu Gly Phe Met Thr Ala Glu Leu Ala Gly
 465 470 475 480
 Val Ile Lys Arg Leu Trp Lys Asp Ser Gly Val Gln Ala Cys Phe Asn
 485 490 495
 Arg Ser Arg Glu Tyr Gln Leu Asn Asp Ser Ala Ala Tyr Tyr Leu Asn
 500 505 510

Asp Leu Asp Arg Ile Ala Gln Pro Asn Tyr Ile Pro Thr Gln Gln Asp
 515 520 525
 Val Leu Arg Thr Arg Val Lys Thr Thr Gly Ile Val Glu Thr His Phe
 530 535 540
 Thr Phe Lys Asp Leu His Phe Lys Met Phe Asp Val Gly Gly Gln Arg
 545 550 555 560
 Ser Glu Arg Lys Lys Trp Ile His Cys Phe Glu Gly Val Thr Ala Ile
 565 570 575
 Ile Phe Cys Val Ala Leu Ser Asp Tyr Asp Leu Val Leu Ala Glu Asp
 580 585 590
 Glu Glu Met Asn Arg Met His Glu Ser Met Lys Leu Phe Asp Ser Ile
 595 600 605
 Cys Asn Asn Lys Trp Phe Thr Asp Thr Ser Ile Ile Leu Phe Leu Asn
 610 615 620
 Lys Lys Asp Leu Phe Glu Glu Lys Ile Lys Lys Ser Pro Leu Thr Ile
 625 630 635 640
 Cys Tyr Pro Glu Tyr Ala Gly Ser Asn Thr Tyr Glu Glu Ala Ala Ala
 645 650 655
 Tyr Ile Gln Cys Gln Phe Glu Asp Leu Asn Lys Arg Lys Asp Thr Lys
 660 665 670
 Glu Ile Tyr Thr His Phe Thr Cys Ala Thr Asp Thr Lys Asn Val Gln
 675 680 685
 Phe Val Phe Asp Ala Val Thr Asp Val Ile Ile Lys Asn Asn Leu Lys
 690 695 700
 Asp Cys Gly Leu Phe
 705